Laminar diffusion combustion

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- Examples of diffusion combustion
  - Jet flame
  - Bunsen burner outer-cone flame
  - Candle flame
- Diffusion flame application
  - Understanding of soot formation
  - NOx and CO emissions control
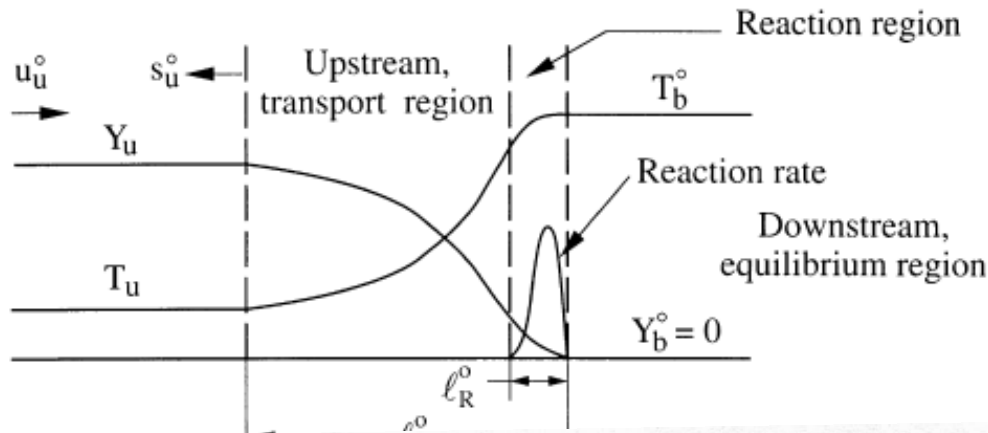 - Flame size and shape control
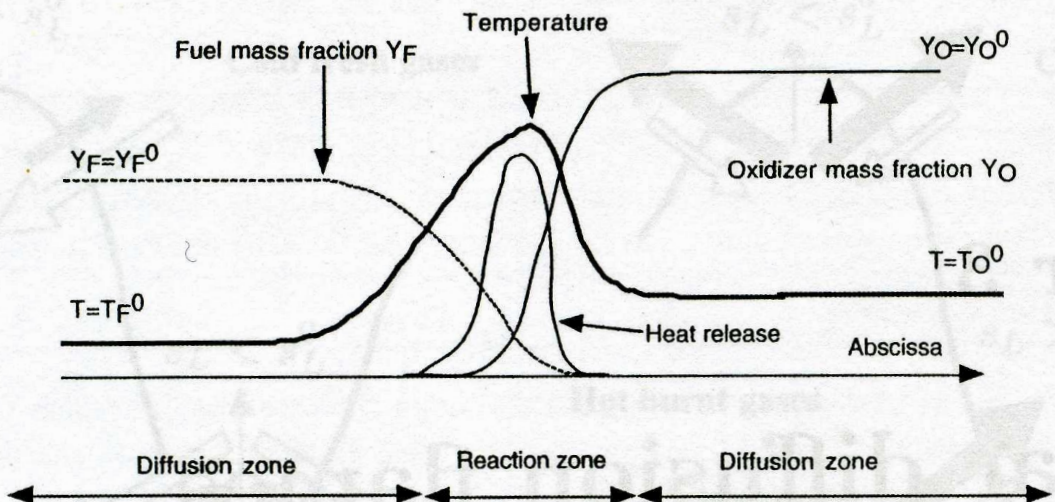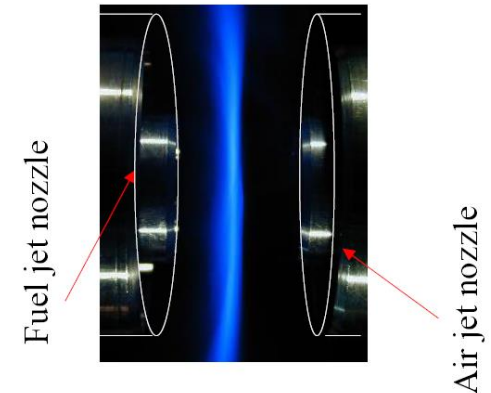- Difference between premixed and diffusion flames

The structure of nonpremixed flame consists of three zones, with a reaction zone separating a fuel-rich zone and oxidizer-rich zone.

C.K Law, Combustion Physics, 2006

Jet flame

Candle flame

Bunsen outer flame

Premixed flame

Non-premixed flame

Fuel jet nozzle

Air jet nozzle

Physical description

Consider a simple case of a non-reacting laminar jet of fuel flowing into an infinite reservoir of oxidiser.

- Figure illustrate of a fuel jet issuing from a nozzle of radius R into still air. Assume the velocity profile is uniform at the tube exit.

- Close to the nozzle, there exists a region call **potential core**, in which both the velocity and nozzle fluid mass fraction remain unchanged.

- In the region between the potential cone and the jet edge, both the velocity and the fuel concentration decrease to zero at the edge of the jet.

- Momentum conserved.
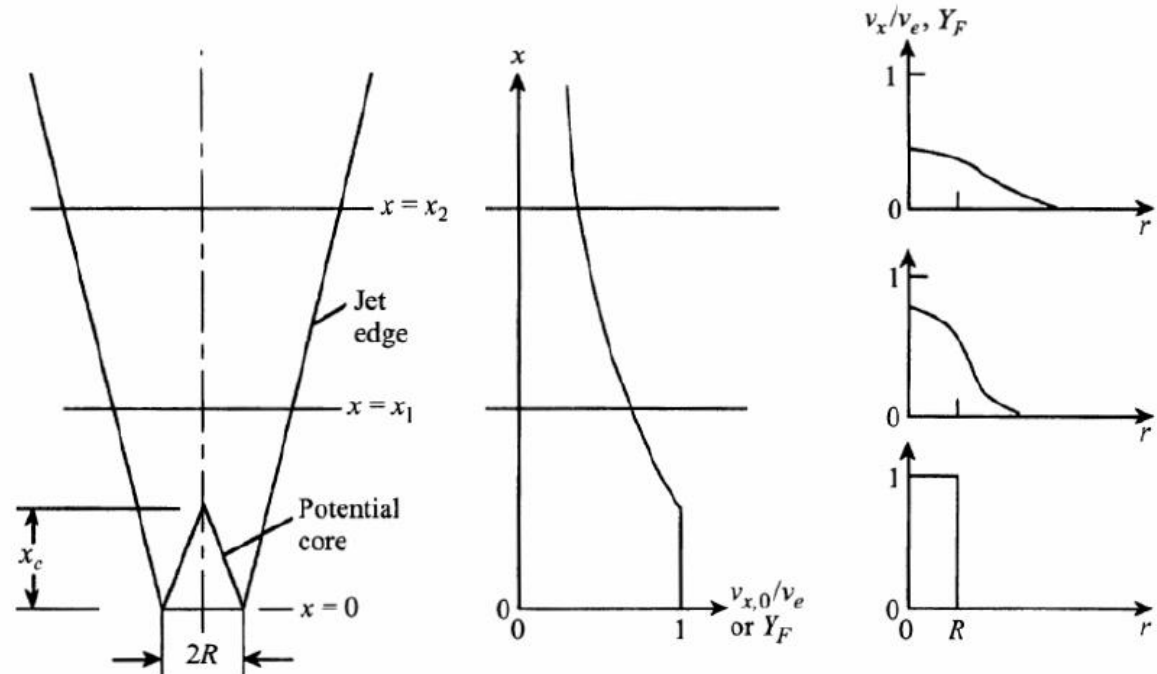
Physical description

Momentum conservation

| Momentum flow of the jet at any x, J | = | Momentum flow issuing from the nozzle, J_e |

$$2\pi \int_0^\infty \rho(r,x)v_x^2(r,x)r\,dr \quad = \quad \rho_e v_e^2 \pi R^2$$

Where ρ_e and v_e are the density and velocity of the fuel at the nozzle exit respectively.

The distribution of the fuel mass fraction $Y_F(r,x)$ should be similar to the velocity destrbution, as shown in the figure last slide.

The mass of the fluid issuing from the nozzle is conserved as well:

$$2\pi \int_0^\infty \rho(r,x)v_x(r,x)Y_F(r,x)r\,dr = \rho_e v_e \pi R^2 Y_{F,e}$$

Where $Y_{F,e} = 1$

Assumptions

Assumptions are made to simplify the determination of velocity and mass fraction distribution

1. The molecular weights of the jet and reservoir fluids are equal -- a uniform fluid density throughout the flow-field.

2. Species molecular transport is by simple binary diffusion governed by Fick's law.

3. Momentum and species diffusivities are constant and equal; thus the **Schmidt number, $S_C \equiv \nu/D$,** is unity.

4. Only radial diffusion of momentum and species is important; axial diffusion is neglected. This implies that the solution only applies some distance downstream of the nozzle exit, because near the exit (too close), axial diffusion is important.

Conservation laws

Mass conservation

$$\frac{\partial v_x}{\partial x} + \frac{1}{r}\frac{\partial (v_r r)}{\partial r} = 0.$$

Axial momentum conservation

$$v_x \frac{\partial v_x}{\partial x} + v_r \frac{\partial v_x}{\partial r} = v\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_x}{\partial r}\right).$$

Species conservation

$$v_x \frac{\partial Y_F}{\partial x} + v_r \frac{\partial Y_F}{\partial r} = D\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial Y_F}{\partial r}\right).$$

Since only two species, fuel and oxidiser, the mass fractions of the two must sum to unity, i.e.

$$Y_{OX} = 1 - Y_F$$

Boundary conditions

We aim to solve the previous equations for the unknown functions, $v_x(r, x)$, $v_r(r, x)$, and $Y_F(r, x)$. This requires boundary conditions.

Along the jet centreline (r=0)

$$v_r(0, x) = 0$$

$$\frac{\partial v_x}{\partial r}(0, x) = 0$$

$$\frac{\partial Y_F}{\partial r}(0, x) = 0$$

At the large radii $r \to \infty$
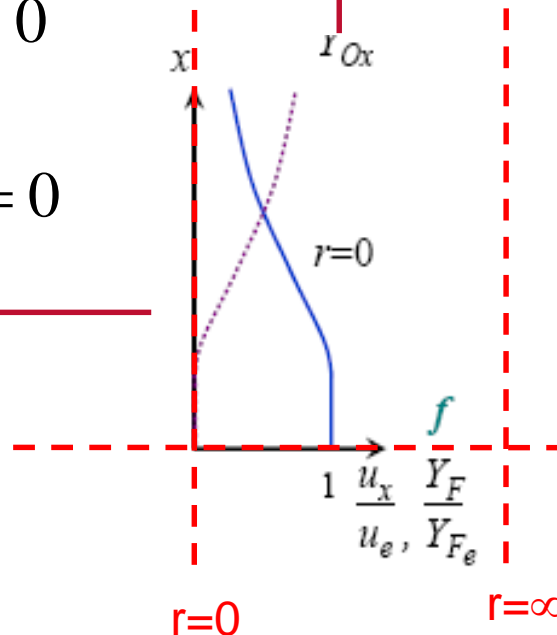
$$v_x(\infty, x) = 0$$

$$Y_F(\infty, x) = 0$$

At the jet exit $x = 0$

$$v_x(r \leq R, 0) = v_e,$$

$$v_x(r > R, 0) = 0,$$

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

$$Y_F(r > R, 0) = 0.$$

Solution

The velocity field can be obtained by assuming the profiles to be similar. The idea of similarity is that the intrinsic shape of the velocity profiles is the same everywhere in the flow field.

For the present problem, this means that the radial distribution of $v_x(r, x)$, is a universal function that depends only on the **similarity variables**, r/x, when normalised by the local centreline velocity $v_x(0, x)$.

The solution for the axial and radial velocities is:

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

$$v_r = (\frac{3J_e}{16\pi\rho_e})^{1/2} \frac{1}{x} \frac{\xi - \frac{\xi^4}{4}}{(1 + \frac{\xi^2}{4})^2},$$

Where J_e is the jet initial momentum flow

$$J_e = \rho_e v_e^2 \pi R^2,$$

And ξ contains the similarity variable r/x

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

Solution

The axial velocity distribution in dimensionless form is

$$v_x / v_e = 0.375(\rho_e v_e R / \mu)(x/R)^{-1}[1 + \xi^2/4]^{-2},$$

The dimensionless centreline velocity decay is obtained by setting r=0 ($\xi = 0$)

$$v_{x,0} / v_e = 0.375(\rho_e v_e R / \mu)(x/R)^{-1}$$
$$= 0.375\, \mathrm{Re}_j (x/R)^{-1}$$

From which we can see that the velocity decays inversely with axial distance and proportional to the jet Reynold number.
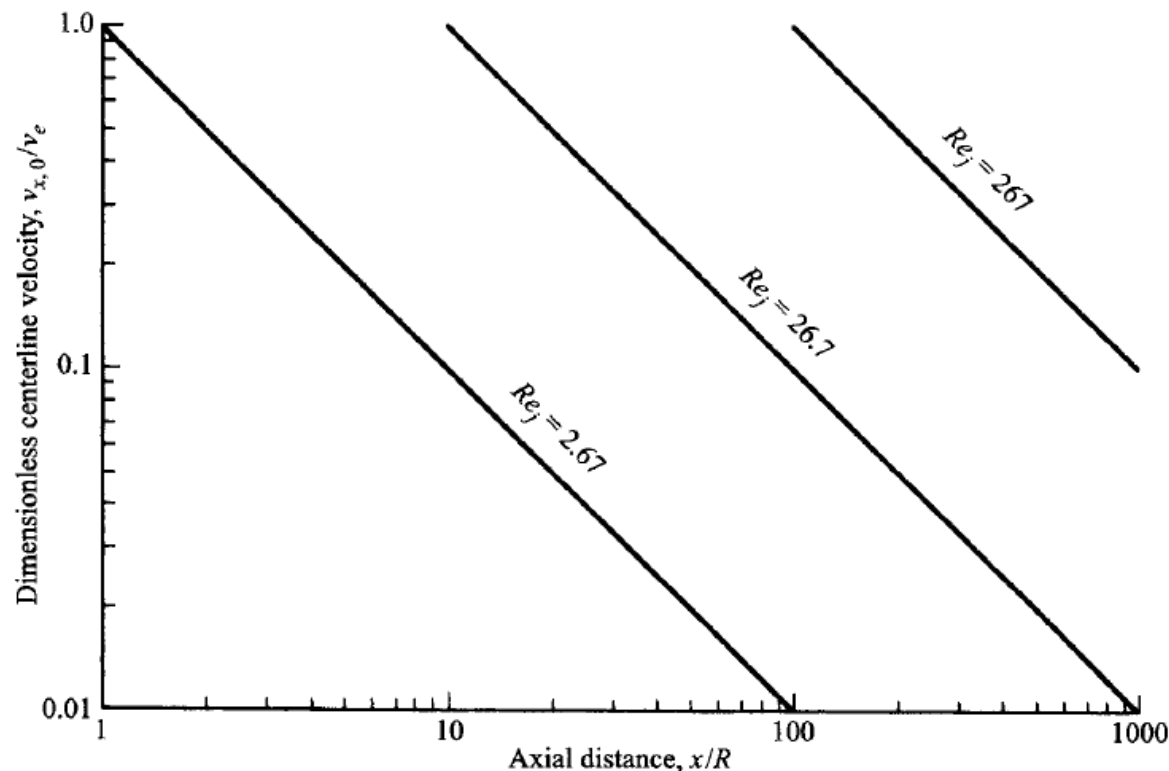
Also this solution is not valid near the nozzle since $v_{x,0}/v_e$ should not exceed 1.

Solution

We also see the centreline velocity decay is more rapid with lower Reynold number jets.

This occurs because as the Re number is decreased, the relative importance of the initial jet momentum becomes smaller in comparison with the viscous shearing action that slows the jet.

Other parameters

We here define **spreading rate** and **spreading angle, α**, and jet **half-width, $r_{1/2}$**

- Jet half-width is the radial location where the jet velocity decayed to half of its centreline value.
- The ratio of the jet half-width to the axial distance x is termed the jet spreading rate.
- The spreading angle is the angle whose tangent is the spreading rate.

$$r_{1/2}/x = 2.97 \left(\frac{\mu}{\rho v_e R} \right) = 2.97 \mathrm{Re}_j^{-1}$$

And

$$\alpha \equiv \tan^{-1}(r_{1/2}/x)$$

These two equations suggest that high Re jets are narrow, and low Re jets are wide.
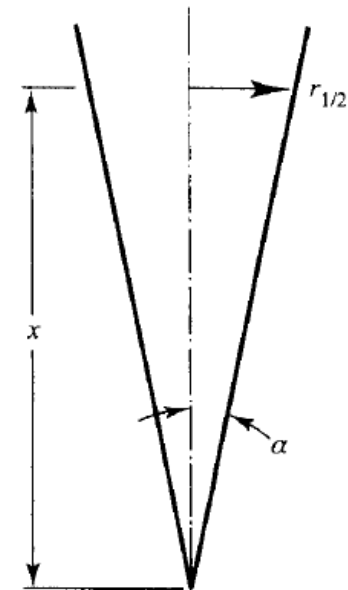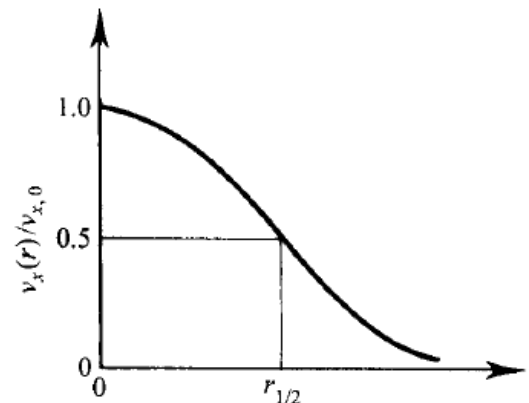
Concentration field

From the previous equations, we notice the fuel mass fraction Y_F and the dimensionless axial velocity v_x/v_e play the same mathematical role, if $Sc = v/D = 1$

$$v_x \frac{\partial v_x}{\partial x} + v_r \frac{\partial v_x}{\partial r} = v \frac{1}{r} \frac{\partial}{\partial r}(r \frac{\partial v_x}{\partial r}).$$

$$v_x \frac{\partial Y_F}{\partial x} + v_r \frac{\partial Y_F}{\partial r} = D \frac{1}{r} \frac{\partial}{\partial r}(r \frac{\partial Y_F}{\partial r}).$$

So the functional form of the solution for Y_F is identical to v_x/v_e

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

Where Q_F is the volumetric flow rate of fuel from the nozzle ($Q_F = v_e \pi R^2$)

As $Sc = v/D = 1$, we have

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

And for the centreline values of the mass fraction

$$Y_F = 0.375 Re_j \left(\frac{x}{R}\right)^{-1}$$

This solution can only apply far from the nozzle, $(x/R) \gtrsim 0.375 Re_j$

A jet of ethylene (C_2H_4) exits a 10-mm-diameter nozzle into still air at 300 K and 1 atm. Compare the spreading angles and axial location where the jet centreline mass fraction drops to the stoichiometric value for initial jet velocities of 10 cm/s and 1.0 cm/s. The viscosity of ethylene at 300 K is $102.3 \times 10^{-7}\ N-s/m^2$.

Since the molecular weighs of C_2H_4 and air are nearly the same, we assume the constant density jet solution can be applied to this problem. Designating 10 cm/s as case 1 and 1 cm/s as case 2.

$$Re_{j,1} = \frac{\rho v_{e,1} R}{\mu} = \frac{1.14(0.1)0.005}{102.3 \cdot 10^{-7}} = 55.7$$

$$Re_{j,2} = \frac{\rho v_{e,2} R}{\mu} = \frac{1.14(0.01)0.005}{102.3 \cdot 10^{-7}} = 5.57$$

Where the density has been determined by ideal gas equation

$$\rho = \frac{p}{\left(\frac{R_0 T}{M}\right)} = \frac{101,325}{\left(\frac{8315}{28.05}\right)300} = 1.14 \; kg/m^3$$

The spreading angle is determine by the previous equation

$$\alpha = \tan^{-1}\left[\frac{2.97}{Re_j}\right]$$

Therefore $\alpha_1 = 3.05°$ and $\alpha_2 = 28.1°$

We see that a low velocity jet is much wider, with a spreading angle about nine times larger than for the high velocity jet.

The stoichiometric fuel mass fraction can be calculated as

$$Y_F = \frac{m_F}{m_A + m_F} = \frac{1}{(A/F)_{stoic} + 1}$$

$(A/F)_{stoic}$ for ethylene is 14.7   (revise, how to calculate)

Thus $Y_F = 0.0637$

To fine the axial location where the centreline fuel mass fraction takes on the stoichiometric value, we set $Y_{F,0} = Y_{F,stoic}$ and solve for x

$$x = \left(\frac{0.375 Re_j}{Y_{F,stoic}}\right) R$$

Therefore, $x_1 = \left(\frac{0.375(55.7)}{0.0637}\right) 0.005 = 1.64 \, m$

$$x_2 = \left(\frac{0.375(5.57)}{0.0637}\right) 0.005 = 0.164 \, m$$

We see that the fuel concentration of the low velocity jet decays to the same value as the high velocity jet in 1/10 the distance.

The burning laminar fuel jet has much in common with isothermal jet.

We first define the flame surface, which is to exist where the fuel and oxidiser meet in stoichiometric proportions.

$$\text{Flame surface} \equiv \left(\begin{array}{l} \text{Locus of points where the} \\ \text{equivalence ratio, } \Phi, \text{ equals unity.} \end{array} \right)$$

Note although the fuel and oxidiser are consumed a the flame, products composition relates to the value of Φ, so the equivalence ratio still has meanings.
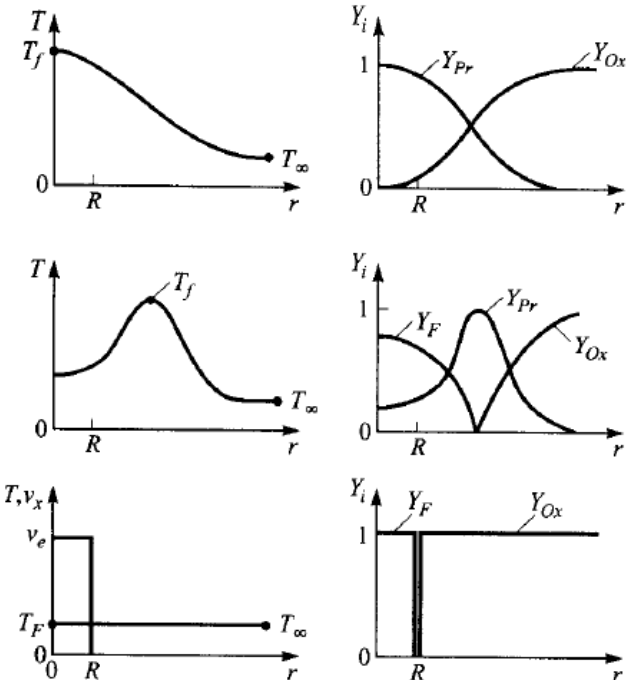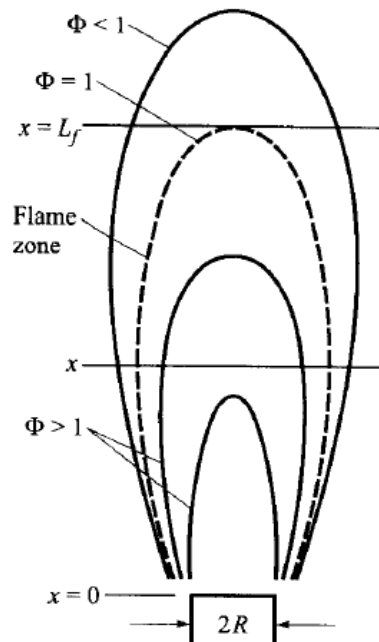
In a jet flame, the products formed at the flame surface diffuse radially both inward and outward. For an **over ventilated** flame, where there is more than enough oxidiser in the surroundings to continuously burn the fuel, we define the flame length L_f by the axial location where

$$\Phi(r = 0, x = L_f) = 1$$

Chemical reactions occur in a narrow region. High temperature reaction zone is an annulus region until the flame tip is reached.
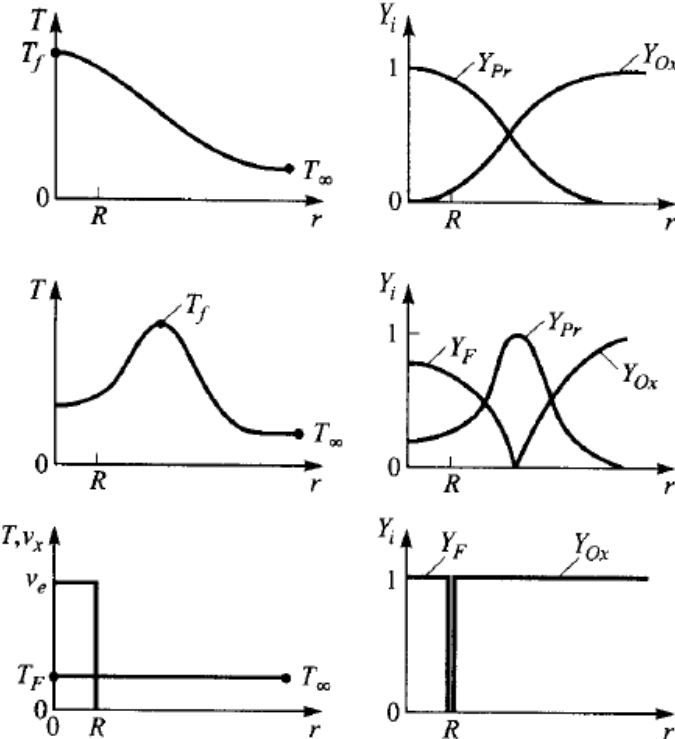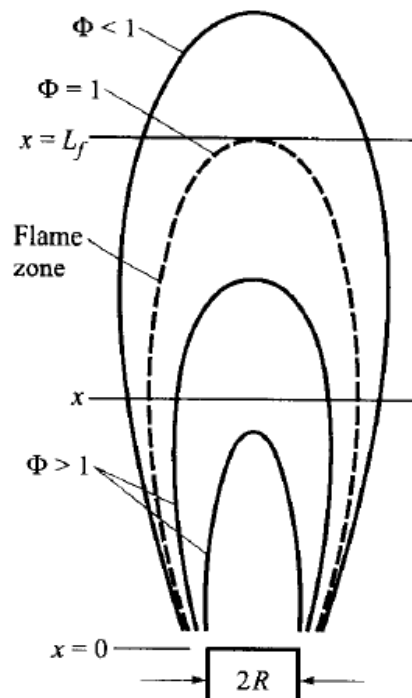
- In the upper regions of a vertical flame, there is a sufficient quantity of hot gases that buoyant forces become important. Buoyancy accelerates the flow and causes a narrowing of the flame, since conservation of mass requires streamlines to come closer together as the velocity increases.

- The narrowing of the flow increases the fuel concentration gradients dY_F/dr, thus enhancing diffusion.

which two

- These two effects tend to cancel each other thus simple theories that neglect buoyancy are able to predict flame lengths reasonably well.
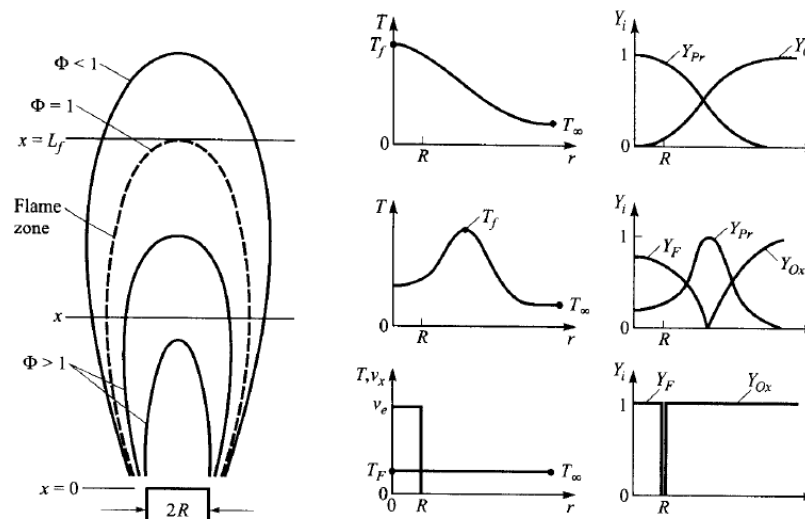
Soot

- For hydrocarbon flames, soot is frequently present, which gives the flame its typical orange or yellow colour.

- Soot is formed on the fuel side of the reaction zone and consumed when flows into the oxidising zone.

- Not all the soot may be oxidised in the high temperature oxidising regions, depending on the fuel type and flame residence time. In this case, soot "wings" may appears, and this soot breaks through is referred to as **smoke**.
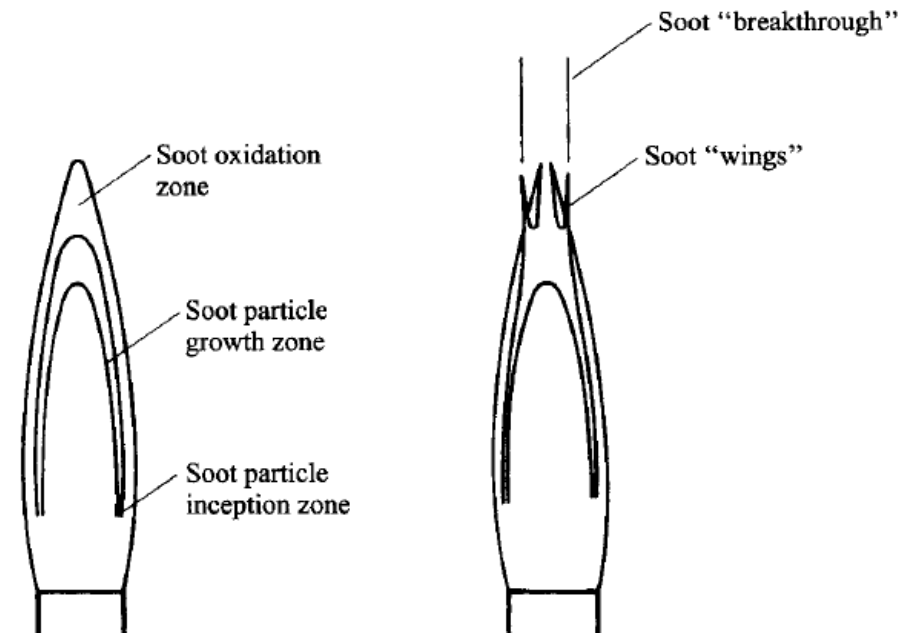
Relationship between flame length and initial conditions

- For circular port flames, the flame length does not depend on initial velocity or diameter but on the initial volumetric flowrate, Q_F. As $Q_F = v_e \pi R^2$, various combination of v_e and R can yield the same flame length.

- From the equation $Y_F = \frac{3}{8\pi} \frac{Q_F}{Dx} \left[1 + \frac{\xi^2}{4}\right]^{-2}$, if ignore the effect of heat release, the equation provides a crude description of the flame boundaries when Y_F is set equal to $Y_{F,stoic}$. Flame length is obtained when r equals zero

$$L_f \approx \frac{3}{8\pi} \frac{Q_F}{D Y_{F,stoic}}$$

- We see from this equation that flame length is proportional to the volumetric flowrate, and inversely proportional to the stoichiometric fuel mass fraction.
- Fuels require less air for complete combustion produce shorter flames

- The formation and destruction of soot is an important feature of non-premixed hydrocarbon-air flames.

- The incandescent soot within the flame is the primary source of a diffusion flame's luminosity.

- Soot also contributes to radiant heat losses from flames, with peak emission at wavelengths in the infrared region.

- In practice, soot formation is to be avoided but diffusion flame is often used as a research tool of soot formation in combustion systems.
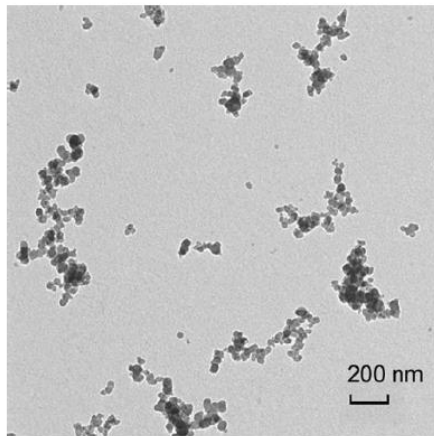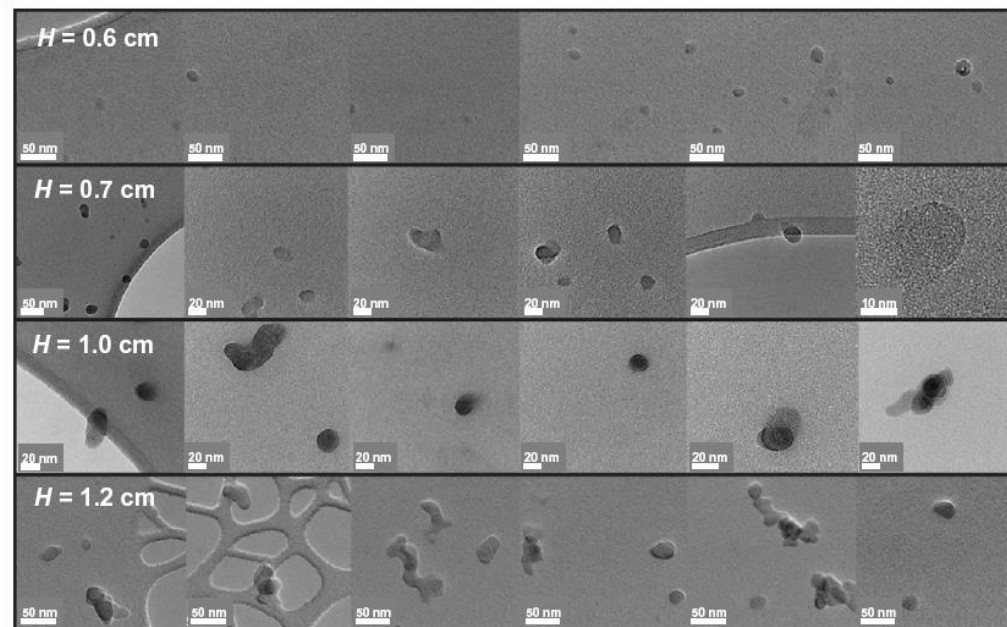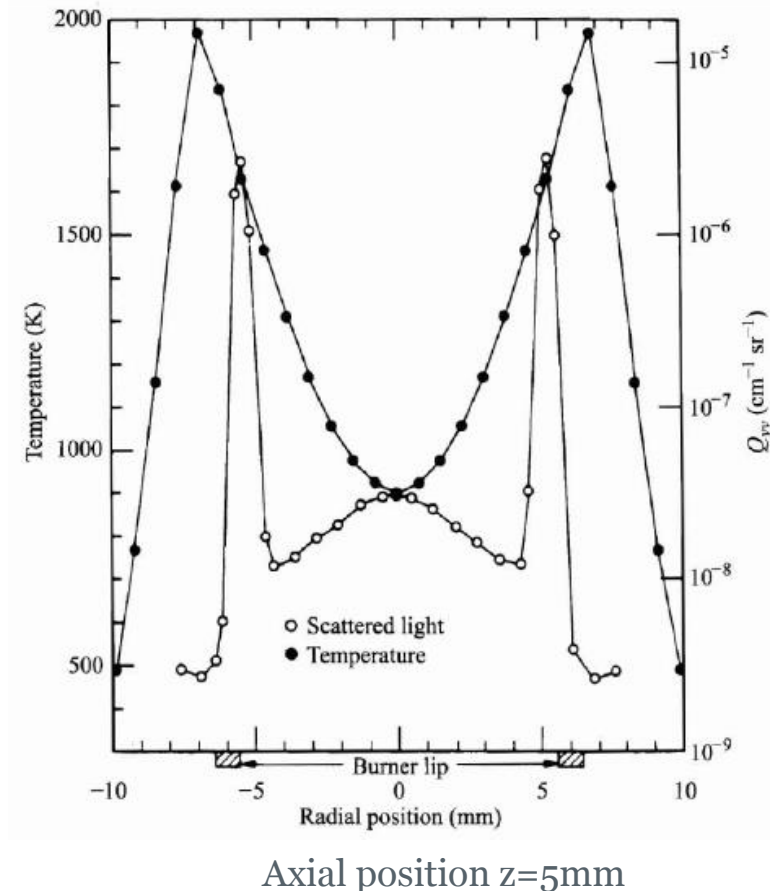
Burner exit

Fig. 4. TEM images of soot particles collected in the burner-stabilized premixed $C_2H_4/O_2/Ar$ flame at $\phi = 2.5$, at several distances H above the burner surface.

Zhao, Uchikawa & Hai Wang; Proc. Combust. Inst. 31 (2007) 851–860

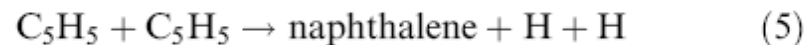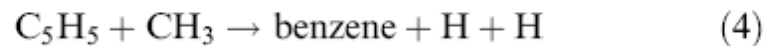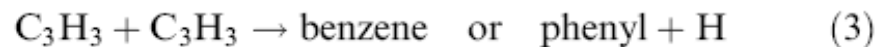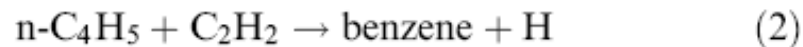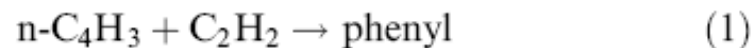- It is generally agreed that soot is formed in diffusion flames over a limited range of temperature, approximately $1300\,K < T < 1600\,K$

- For the temperature profile and light scattered by soot particles, the two peaks correspond to regions containing significant amount of soot.

- Soot peaks are at radial locations interior to the temperature peaks and correspond to temperature of ~1600 K.

- Soot region is very narrow and confined to a restricted range of temperatures.

- Soot formation and destruction process is extremely complex but can be considered:

  - Formation of precursor species
  - Particle inception
  - Surface growth and particle agglomeration
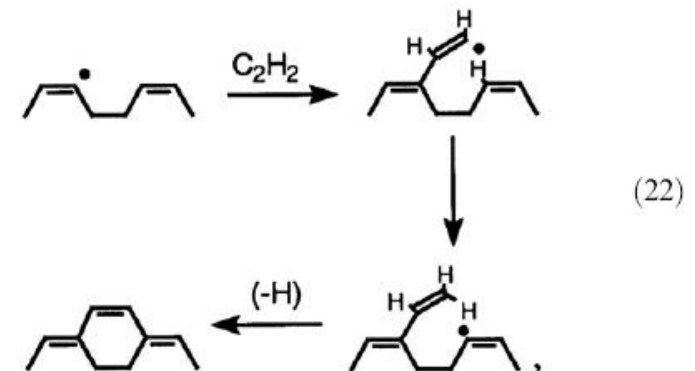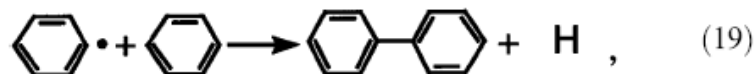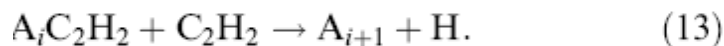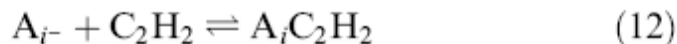 - Particle oxidation

Axial position z=5mm
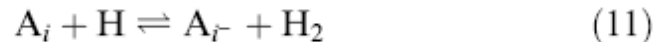
- In the first step, the formation of soot precursor species, polycyclic aromatic hydrocarbon (PAH) are though to be important intermediates between the original fuel molecule and primary soot particle.

- Chemical kinetics plays an important role in the first step.

- The formation of ring structure and their growth via reactions with acetylene (C_2H_2) have been identified as important processes.

1-Formation of aromatics

$$n\text{-}C_4H_3 + C_2H_2 \rightarrow \text{phenyl} \tag{1}$$

$$n\text{-}C_4H_5 + C_2H_2 \rightarrow \text{benzene} + H \tag{2}$$

$$C_3H_3 + C_3H_3 \rightarrow \text{benzene} \quad \text{or} \quad \text{phenyl} + H \tag{3}$$

$$C_5H_5 + CH_3 \rightarrow \text{benzene} + H + H \tag{4}$$

$$C_5H_5 + C_5H_5 \rightarrow \text{naphthalene} + H + H \tag{5}$$

2-Growth of aromatics

$$A_i + H \rightleftharpoons A_{i\text{-}} + H_2 \tag{11}$$

$$A_{i\text{-}} + C_2H_2 \rightleftharpoons A_iC_2H_2 \tag{12}$$

$$A_iC_2H_2 + C_2H_2 \rightarrow A_{i+1} + H. \tag{13}$$

(19)

(22)

- Particle inception step involves the formation of small particles of a critical size (3,000-10,000 atomic mass units) from growth by both chemical means and coagulation.
- In this step, the large molecules are transformed to particles.
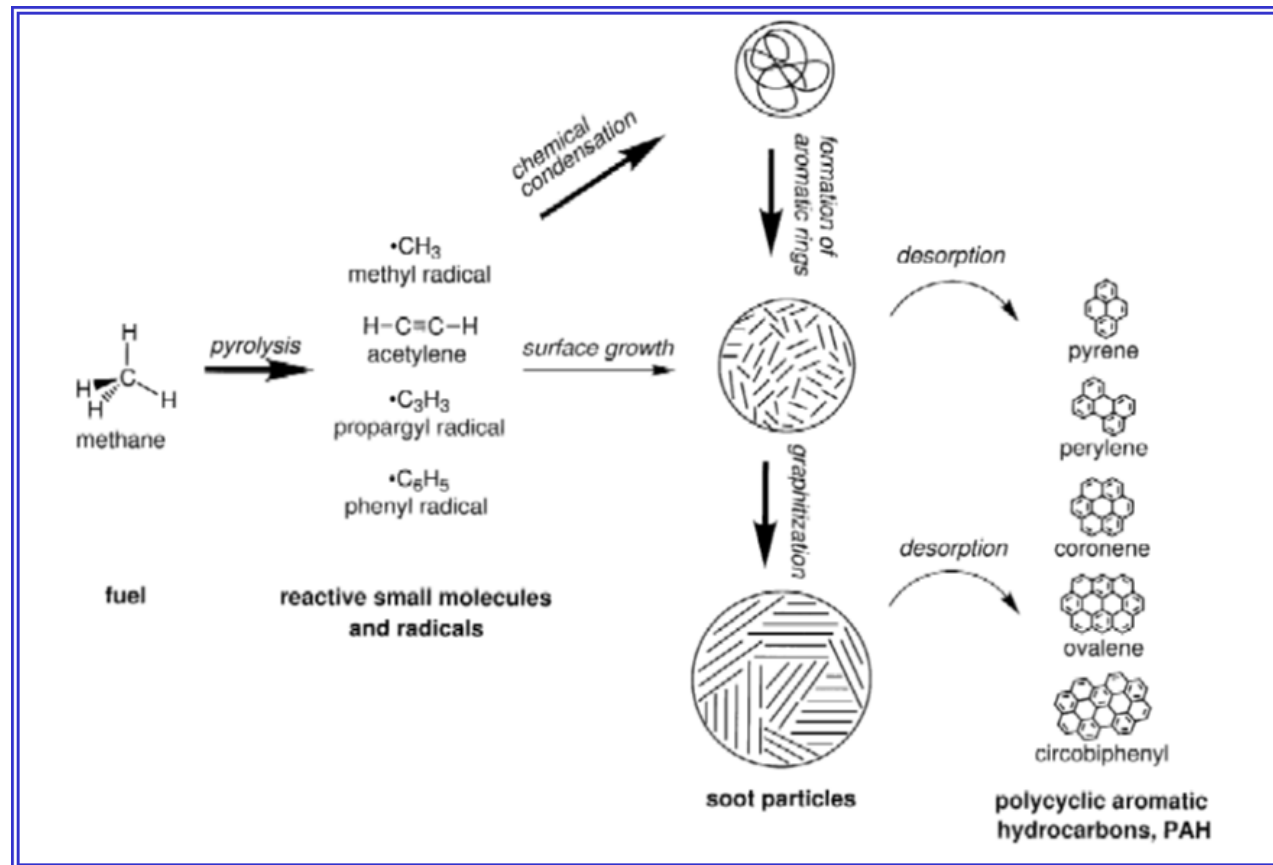
- When small primary soot particles continue to be exposed to the species from the pyrolising fuel as they travel through the flame, they experience surface growth.

- At the same time, they pass through an oxidising region of the flame.
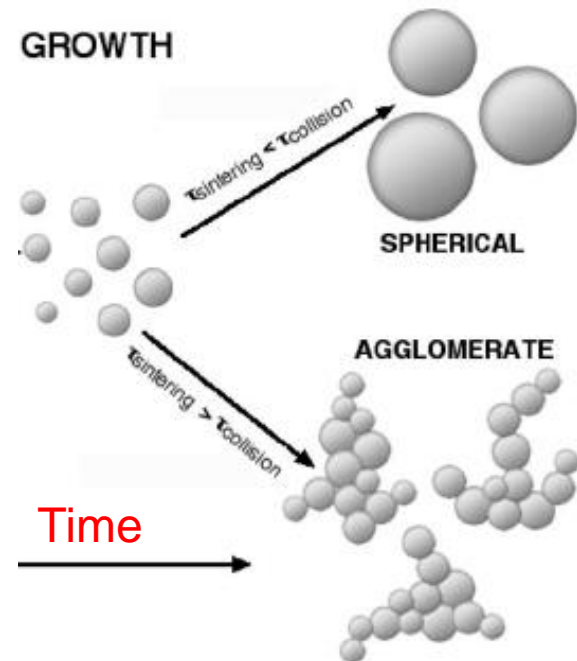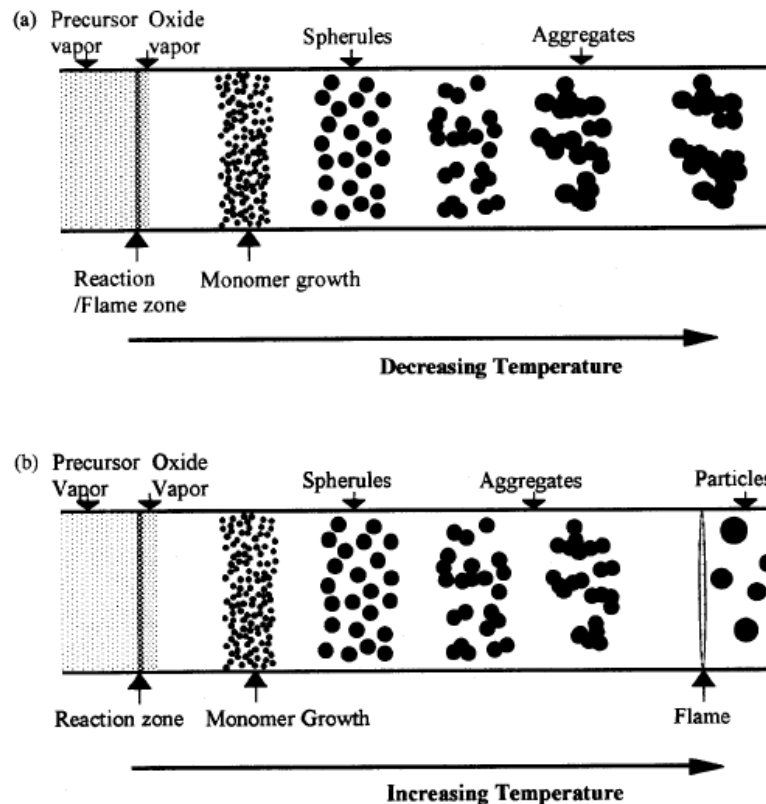
- If all the soot particles are oxidised, the flame is non-sooting. Or incomplete oxidation yields a sooting flame.

- Non-zero of the soot volume fraction beyond the flame tip indicates a sooting flame.

- The amount of soot formed in a diffusion flame is strongly dependent on fuel type.

- An experimentally determined measure of a fuel's tendency to soot is so called "smoke point".

- The basic concept is to increase the fuel flow rate until smoke is observed to escape from the flame tip.
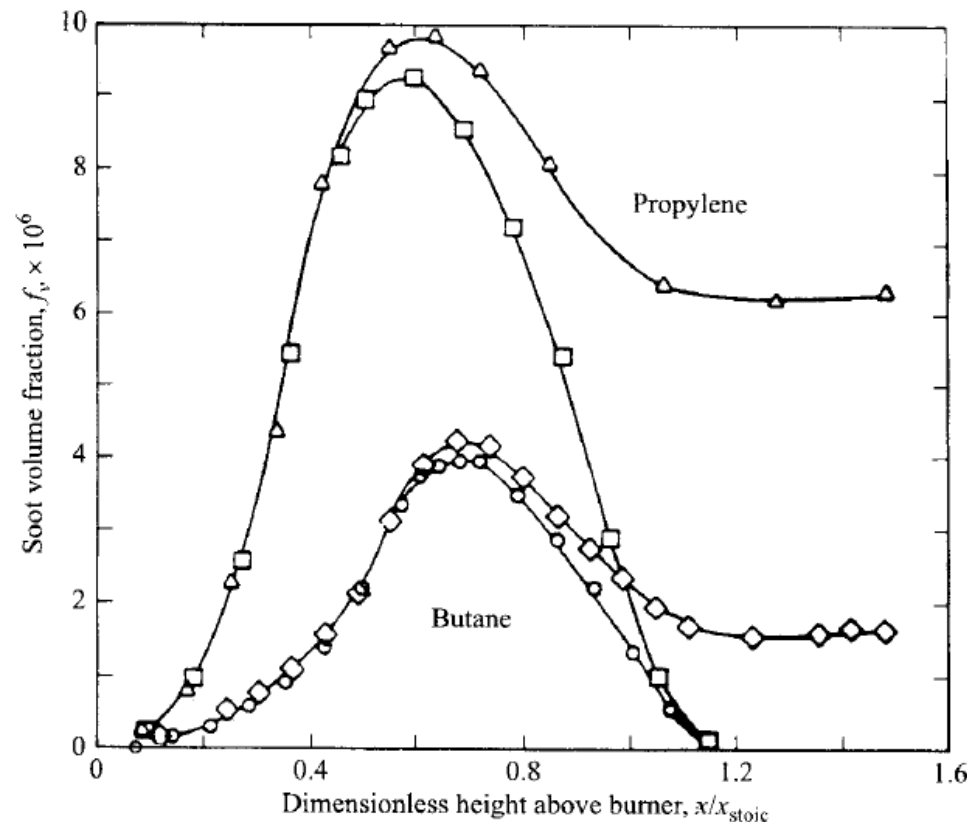
- Greater fuel flowrate at the incipient sooting condition, less sooting propensity.
- The larger flame height at the incipient sooting condition, the lower the sooting propensity.
- Fuel sooting propensity from least to greatest order, is alkanes, alkenes, alkynes, and aromatics. The fuel molecular structure is very important in determining the fuel's sooting propensity.
- Ring compounds and their growth via acetylene are important in soot formation.

Table 9.6   Smoke points by hydrocarbon family[a]

Alkanes		Alkenes		Alkynes		Aliphatic aromatics	
Fuel	$\dot{m}_{sp}$[b]	Fuel	$\dot{m}_{sp}$[b]	Fuel	$\dot{m}_{sp}$[b]	Fuel	$\dot{m}_{sp}$[b]
Propane	7.87	Ethylene	3.84	Acetylene	0.51	Toluene	0.27
Butane	7.00	Propylene	1.12	1-Heptyne	0.65	Styrene	0.22
n-Heptane	5.13	1-Octene	1.73	1-Decyne	0.80	o-Xylene	0.28
Isooctane	1.57	1-Decene	1.77			n-Butylbenzene	0.27
		1-Hexadecene	1.93				

[a]SOURCE: Data from Ref. [26].
[b]Smoke point flowrate in mg/s.

- Laminar non-reaction jet and simplified solution
- Boundary conditions for jet flow
- Jet flame and its physical description
- Soot formation and destruction