

Combustion Theory premixed and diffusion flames part (1)

Overview of Combustion

Ignition

Three things must be present at the same time in order to produce fire:

- Enough oxygen to provide combustion
- Enough heat to raise the material temperature to its ignition temperature
- **Fuel** or combustible material which produces high **exothermic reaction** to propagate heat to not-yet- burnt material nearby





Introduction

Basic Flame Types:

- Premixed flames: fuel and oxidizer are homogeneously mixed before reaction occurs. Laminar and turbulent premixed flames
- Non premixed flames: fuel and oxidizer come into contact during combustion process. Laminar and turbulent diffusion flames





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1. Laminar premixed flames

- Premixed combustion used in combustion devices when high heat release rates are desired
 - Small devices
 - Low residence times
- Examples:
 - SI engine
 - Stationary gas turbines
- Advantage → Lean combustion possible
 - Smoke-free combustion
 - Low NO_x
- Disadvantage: Danger of
 - Explosions
 - Combustion instabilities
 - → Large-scale industrial furnaces and aircraft engines are typically non-premixed





Laminar premixed flames

A premixed flame is a self-sustaining propagation of a localized combustion zone at subsonic velocities (deflagration regime)

The classical device to generate a laminar premixed flame is the Bunsen burner:





Typical Bunsen burner flame

Example: Typical Bunsen-burner CH₄/Air flame



Typical Bunsen-burner flame is a dual flame:

- a fuel-rich premixed inner flame
- a diffusion outer flame: CO and H₂ from inner flame encounter ambient air

• Experimental evidence for the presence of a cool inner preheating region



A wire to reveal the presence of a cool preheating region containing unburned CH_4 and O_2



A match in preheating region does not ignite until it is moved to the inner cone

•	Basic 1	features	of	laminar	premixed	flames
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Fuel/Air Ratio	Fuel lean	Stochiometric	Fuel rich	Very fuel rich
Flame colour, <i>i.e. colour of the</i> outer cone	Deep Violet due to large concentrations of excited CH radicals	Blue	Green due to large concentrations of C_2 species	Yellow due to carbon particles
			High-T burned gases usually show a reddish glow due to radiation from CO_2 and H_2O	

Flame characteristics for hydrocarbon-air stoichiometric mixtures

- The flame is ~1 mm thick and moves at ~0.5 m/s
- Pressure drop through the flame is very small: ~1 Pa
- Temperature in reaction zone is ~2200-2600 K
- Density ratio of reactants to products is ~7

• Kinematic balance for a steady oblique flame



Laminar Bunsen flame

Thermal expansion the flame front

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• Normal component of velocity vector

$$(\rho v_n)_u = (\rho v_n)_b$$
 $v_{n,b} = v_{n,u} \frac{\rho_u}{\rho_b}$

- Tangential component of velocity vector $v_{t,u} = v_{t,b}$
- At steady-state the burning velocity equals the flow velocity of the unburnt mixture normal to the flame front

$$S_{L,u} = v_{n,u} = v_u \sin \alpha$$

2- Turbulent flames

- Most of combustion devices operate in turbulent flow regime, i.e. internal combustion or aircraft engines, industrial burners and furnaces. Laminar combustion applications are almost limited to candles, lighters and some domestic furnaces. Turbulence increases the mixing processes thus enhancing combustion.
- Also combustion influences turbulence. Heat release due to combustion causes very strong flow accelerations through the flame front (flamegenerated turbulence). Moreover, huge changes in kinematic viscosity associated with temperature changes may damp turbulence leading to flow relaminarization



Turbulence

- Combustion requires mixing at the molecular level
- Turbulence: convective transport \uparrow \rightarrow molecular mixing \uparrow



Turbulent shear flows

- Relevant flow cases in technical systems
 - Round jet
 - Flow around airfoil
 - Flows in combustion chamber
- Due to the complexity of these turbulent flows they cannot be described theoretically





"Temporally evolving shear layer": Scalar dissipation rate χ (left), mixture fraction Z (rechts)



Turbulent jet: magnitude of vorticity



Structure of a one-dimensional premixed laminar flame.



Structure of a one-dimensional non-premixed laminar flame. Here fuel and oxidizer streams are assumed to have the same temperature.

LAMINAR PREMIXED FLAMES

OVERVIEW

Applications:

- Heating appliances
- Bunsen burners
- Burner for glass product manufacturing

Importance of studying laminar premixed flames:

- Some burners use this type of flames as shown by examples above
- Prerequisite to the study of turbulent premixed flames. Both have the same physical processes and many turbulent flame theories are based on underlying laminar flame structure.

PHYSICAL DESCRIPTION

Physical characteristics

- Figure 8.2 shows typical flame temperature profile, mole fraction of reactants, χ_R , and volumetric heat release, $.\dot{Q}''$
- Velocity of reactants entering the flame, v_u = flame propagation velocity, S_L
- Products heated ⇒ product density (ρ_b) < reactant density (ρ_u). Continuity requires that burned gas velicity, ν_b >= unburned gas vel., ν_u

 $\rho_{\rm u} v_{\rm u} A = \rho_{\rm b} v_{\rm b} A \qquad (8.1)$

For a typical hydrocarbon-air flame at P_{atm}, ρ_u/ρ_b ~ 7 ⇒ considerable acceleration of the gas flow across the flame (v_b to v_u).



A flame consists of 2 zones:

Preheat zone, where little heat is released

Reaction zone, where the bulk of chemical energy is released

Reaction zone consists of 2 regions:

Thin region (less than a millimeter), where reactions are very fast

• Wide region (several millimeters), where reactions are slow

- In thin region (fast reaction zone), destruction of the fuel molecules and creation of many intermediate species occur. This region is dominated by bimolecular reactions to produce CO.
- Wide zone (slow reaction zone) is dominated by radical recombination reactions and final burnout of CO via CO + OH \rightarrow CO₂ +H

Flame colours in fast-reaction zone:

- If air > stoichiometric proportions, excited CH radicals result in blue radiation.
- If air < stoichiometric proportions, the zone appears blue-green as a result of radiation from excited C₂.

In both flame regions, OH radicals contribute to the visible radiation, and to a lesser degree due to reaction $CO + O \rightarrow CO_2 + hv$.

If the flame is fuel-rich (much less air), soot will form, with its consequent blackbody continuum radiation. Although soot radiation has its maximum intensity in the infrared (recall Wien's law for blackbody radiation), the spectral sensitivity of the human eye causes us to see a bright yellow (near white) to dull orange emission, depending on the flame temperature



Spectrum of flame colours

Typical Laboratory Premixed Flames:-

- The typical Bunsen-burner flame is a dual flame: a fuel rich premixed inner flame surrounded by a diffusion flame. illustrates a Bunsen burner.
- The diffusion flame results when CO and OH from the rich inner flame encounter the ambient air.
- The shape of the flame is determined by the combined effects of the velocity profile and heat losses to the tube wall.

• For the flame to remain stationary, $S_L = normal component of v_u = v_u sin\alpha$ (8.2). Figure 8.3b illustrates vector diagram.



Figure 8.3 (a) Bunsen-burner schematic. (b) Laminar flame speed equals normal component of unburned gas velocity, $v_{u,n}$.

Fuel & Advanced Combustion

Lecture LAMINAR PREMIXED FLAMES PART (2)

SIMPLIFIED ANALYSIS

Turns (2000) proposes simplified laminar flame speed and thickness on one-dimensional flame. Assumptions used:

One-dimensional, constant-area, steady flow.
 One-dimensional flat flame is shown in Figure 8.5.

Kinetic and potential energies, viscous shear work, and thermal radiation are all neglected.

The small pressure difference across the flame is neglected; thus, pressure is constant.



Fgure 8.5 (a) Adiabatic flat-flame burner. (b) Nonadiabatic flat-flame burner.

- The diffusion of heat and mass are governed by Fourier's and Fick's laws respectively (laminar flow).
- Binary diffusion is assumed.
 - The Lewis number, Le, which expresses the ratio of thermal diffusivity, α, to mass diffusivity, D, i.e.,
 is unity,

$$Le = \frac{\alpha}{D} = \frac{k}{\rho C_p D}$$

$$\alpha = \frac{k}{\rho_u C_p}$$

The Cp mixture ≠ f(temperature, composition). This is equivalent to assuming that individual species specific heats are all equal and constant.

Fuel and oxidizer form products in a single-step exothermic reaction. Reaction is
 1 kg fuel + v kg oxidiser → (v + 1)kg products

The oxidizer is present in stoichiometric or excess proportions; thus fuel is completely consumed at the flame. • For this simplified system, S_L and δ found are

$$S_{L} = \left[-2\alpha\left(\nu+1\right)\frac{\bar{m}_{F}''}{\rho_{u}}\right]^{1/2}$$

and

$$\delta = \left[\frac{-2\rho_u\alpha}{(\nu+1)\bar{m}_F'''}\right]$$

Or

 $\delta = \frac{2\alpha}{S_I}$



(8.20)

where is \dot{m}_{F}''' volumetric mass rate of fuel and α is thermal diffusivity. Temperature profile is assumed linear from T_u to T_b over the small distance, as shown in Fig. 8.9.



Figure 8.9

Assumed temperature profile for laminar premixed flame analysis.

FACTORS INFLUENCING FLAME SPEED (S_L) AND FLAME THICKNESS (δ)

1. Temperature (T_{μ} and T_{b})

• Temperature dependencies of S_1 and δ can be inferred from Eqns 8.20 and 8.21. Explicit dependencies is proposed by Turns as follows

 $\square \alpha \propto \frac{k(T)}{\rho_{\mu}C_{p}(\overline{T})} \propto \overline{T}^{0.75} T_{\mu}P^{-1}$ (8.27)

where α is thermal diffusivity, T_u is unburned gas temperature, $\overline{T} \equiv 0.5(T_b + T_u)$, T_b is burned gas temperature.

where the exponent n is the overall reaction order, $R_u =$ universal gas constant (J/kmol-K), $E_A =$ activation energy (J/kmol)

Combining above scalings yields and applying Eqs 8.20 and 8.21

■ <mark>S_L ∞ (8.29)</mark>

 $\bullet \delta \propto$

$$\overline{T}^{0.375} T_{u} T_{b}^{-n/2} \exp\left(\frac{-E_{A}}{2R_{u} T_{b}}\right) \left(\frac{8}{p}, \frac{30}{2}\right)$$

$$\overline{T}^{0.375} T_{b}^{n/2} \exp\left(\frac{E_{A}}{2R_{u} T_{b}}\right) P^{-n/2}$$

- For hydrocarbons, n ≈ 2 and E_A ≈ 1.67.10⁸ J/kmol (40 kcal/gmol). Eqn 8.29 predicts S_L to increase by factor of 3.64 when T_u is increased from 300 to 600K. Table 8.1 shows comparisons of S_L and δ
- The empirical S_L correlation of Andrews and Bradley [19] for stoichiometric methane-air flames,
 S_L (cm/s) = 10 + 3.71.10⁻⁴[T_u(K)]² (8.31) which is shown in Fig. 8.13, along with data from several experimenters.
- Using Eqn. 8.31, an increase in T_u from 300 K to 600 K results in S_L increasing by a factor of 3.3, which compares quite favourably with our estimate of 3.64 (Table 8.1).





Table 8.1 Estimate of effects of T_u and T_b on S_L and δ using Eq 8.29 and 8.30

Case	A (ref)	B	C
T _u (K)	300	600	300
T _b (K)	2,000	2,300	1,700
S _L /S _{L,A}	1	3.64	0.46
δ/δ_A	1	0.65	1.95

Case A: reference

- Case C: T_b changes due to heat transfer or changing equivalent ratio, either lean or rich.
- Case B: T_u changes due to preheating fuel

Pressure (P)

- From Eq. 8.29, if, again, $n \approx 2$, $S_L \neq f$ (P).
- Experimental measurements generally show a negative dependence of pressure. Andrews and Bradley [19] found that
 - S_{L} (cm/s) = 43[P (atm)]^{-0.5} (8.32)

fits their data for P > 5 atm for methane-air flames (Fig. 8.14).





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Equivalent Ratio (Φ)

- Except for very rich mixtures, the primary effect of Φ on S_L for similar fuels is a result of how this parameter affects flame temperatures; thus, we would expect S_{L,max} at a slightly rich mixture and fall off on either side as shown in Fig. 8.15 for behaviour of methane.
- Flame thickness (δ) shows the inverse trend, having a minimum near stoichiometric (Fig. 8.16).

Fuel Type

- Fig. 8.17 shows S_L for C₁-C₆ paraffins (single bonds), olefins (double bonds), and acetylenes (triple bonds). Also shown is H₂. S_L of C₃H₈ is used as a reference.
- Roughly speaking the C₃-C₆ hydrocarbons all follow the same trend as a function of flame temperature. C₂H₄ and C₂H₂' S_L > the C₃-C₆ group, while CH₄'S_L lies somewhat below.



Figure 8.15 Effect of equivalence ratio on the laminar flame speed of methane-air mixtures at atmospheric pressure. SOURCE: Reprinted with permission, Elsevier Science, Inc., from Ref. [19], (1972, The Combustion Institute.





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Figure 8.17 Relative flame speeds for C_1-C_6 hydrocarbon fuels. The reference flame speed is based on propane using the tube method [21].

- H_2 's $S_{L,max}$ is many times > that of C_3H_8 . Several factors combine to give H_2 its high flame speed:
- i. the thermal diffusivity (α) of pure H₂ is many times > the hydrocarbon fuels;
- ii. the mass diffusivity (D) of H_2 likewise is much > the hydrocarbons;
- iii. the reaction kinetics for H_2 are very rapid since the relatively slow $CO \rightarrow CO_2$ step that is a major factor in hydrocarbon combustion is absent.

 Law [20] presents a compilation of laminar flame-speed data for various pure fuels and mixtures shown in Table 8.2.

Table 8.2 S_L for various pure fuels burning in air for $\Phi = 1.0$ and at 1 atm

Fuel	S _L (cm/s)
CH ₄	40
C_2H_2	136
C ₂ H ₄	67
C ₂ H ₆	43
C ₃ H ₈	44
H ₂	210

FLAME SPEED CORRELATIONS FOR SELECTED FUELS

Metghalchi and Keck [11] experimentally determined S_L for various fuel-air mixtures over a range of temperatures and pressures typical of conditions associated with reciprocating internal combustion engines and gas turbine combustors.
 Eqn 8.33 similar to Eqn. 8.29 is proposed

$$\begin{array}{l} \mathbf{S}_{\mathsf{L}} = \mathbf{S}_{\mathsf{L},\mathsf{ref}} \\ (8.33) \end{array} \quad \left(\frac{T_u}{T_{u,ref}}\right)^{\gamma} \left(\frac{P}{P_{ref}}\right)^{\beta} \quad (1-2.1 \, \mathsf{Y}_{\mathsf{dil}})^{\beta} \end{array}$$

for $T_u > \approx 350$ K.

The subscript ref refers to reference conditions defined by

 $T_{u,ref} = 298 \text{ K}, P_{ref} = 1 \text{ atm and}$

 $S_{L,ref} = B_M + B_2(\Phi - \Phi_M)^2$ (for reference conditions)

where the constants B_M , B_2 , and Φ_M depend on fuel type and are given in Table 8.3.

• Exponents of T and P, γ and β are functions of Φ , expressed as

 $\gamma = 2.18 - 0.8(\Phi - 1)$ (for non-reference conditions)

 $\beta = -0.16 + 0.22(\Phi - 1)$ (for non-reference conditions)

The term Y_{dil} is the mass fraction of diluent present in the air-fuel mixture in Eqn. 8.33 to account for any recirculated combustion products. This is a common technique used to control NO_x in many combustion systems

Table 8.3 Values for B_M , B_2 , and Φ_M used in Eqn 8.33 [11]

Fuel	Φ_{M}	B _M (cm/s)	B ₂ (cm/s)
Methanol	1.11	36.92	-140.51
Propane	1.08	34.22	-138.65
lso octane	1.13	26.32	-84.72
RMFD-303	1.13	27.58	-78.54

Example 8.3

Compare the laminar flame speeds of gasoline-air mixtures with $\Phi = 0.8$ for the following three cases:

- i. At ref conditions of T = 298 K and P = 1 atm
- ii. At conditions typical of a spark-ignition engine operating at wide-open throttle: T = 685 K and P = 18.38 atm.
- iii. Same as condition ii above, but with 15 percent (by mass) exhaust-gas recirculation

Solution

• RMFD-303 research fuel has a controlled composition simulating typical gasolines. The flame speed at 298 K and 1 atm is given by

$$S_{L,ref} = B_M + B_2(\Phi - \Phi_M)^2$$

From Table 8.3,

- $B_M = 27.58 \text{ cm/s}, B_2 = -78.38 \text{cm/s}, \Phi_M = 1.13.$
- $S_{L,ref} = 27.58 78.34(0.8 1.13)^2 = 19.05 \text{ cm/s}$
- To find the flame speed at T_u and P other than the reference state, we employ Eqn. 8.33

$${}^{\bullet}S_{L}(T_{u}, P) = S_{L,ref}$$

$$\left(\frac{T_u}{T_{u,ref}}\right)^{\gamma} \left(\frac{P}{P_{ref}}\right)^{\beta}$$

where $\gamma = 2.18 - 0.8(\Phi - 1) = 2.34$ $\beta = -0.16 + 0.22(\Phi - 1) = -0.204$ Thus, S_{I} (685 K, 18.38 atm) = $19.05 (685/298)^{2.34} (18.38/1)^{-0.204} = 73.8 \text{ cm/s}$ With dilution by exhaust-gas recirculation, the flame speed is reduced by factor $(1-2.1 Y_{dil})$: S_{I} (685 K, 18.38 atm, 15% EGR) = 73.8cm/s[1-2.1(0.15)]= **50.6 cm/s**

QUENCHING, FLAMMABILITY, AND IGNITION

- Previously \$\Rightarrow\$ steady propagation of premixed laminar flames
- Now
 rightarrow transient process: quenching and ignition. Attention to quenching distance, flammability limits, and minimum ignition energies with heat losses controlling the phenomena.

1. Quenching by a Cold Wall

Flames extinguish upon entering a sufficiently small passageway. If the passageway is not too small, the flame will propagate through it. The critical diameter of a circular tube where a flame extinguishes rather than propagates, is referred to as the quenching distance.

 Experimental quenching distances are determined by observing whether a flame stabilised above a tube does or does not flashback for a particular tube diameter when the reactant flow is rapidly shut off. Quenching distances are also determined using high-aspect-ratio rectangular-slot burners. In this case, the quenching distance between the long sides, i.e., the slit width.

 Tube-based quenching distances are somewhat larger (~20-50 percent) than slit-based ones [21]



2. Flammability Limits

A flame will propagate only within a range of mixture the so-called lower and upper limits of flammability. The limit is the leanest mixture (Φ < 1), while the upper limit represents the richest mixture (Φ > 1). Φ = (A/F)_{stoich} /(A/F)_{actual} by mass or by mole

 Flammability limits are frequently quoted as %fuel by volume in the mixture, or as a % of the stoichiometric fuel requirement, i.e., (Φ x 100%). Table 8.4 shows flammability limits of some fuels Flammability limits for a number of fuel-air mixtures at atmospheric pressure is obtained from experiments employing "tube method".

In this method, it is ascertained whether or not a flame initiated at the bottom of a vertical tube (approximately 50-mm diameter by 1.2-m long) propagates the length of the tube.

A mixture that sustains the flame is said to be flammable. By adjusting the mixture strength, the flammability limit can be ascertained.

Table 8.4 Flammability limits, quenching distances and minimum ignition energies

	Flammability limit			Quenching distance, d	
	$\Phi_{\sf min}$	Φ_{max}	Stoich-mass	For ⊕=1	Absolute
			air-fuel ratio		min, mm
C_2H_2	0.19	∞	13.3	2.3	-
CO	0.34	6.76	2.46	-	-
C ₁₀ H ₂₂	0.36	3.92	15.0	2.1	-
C_2H_6	0.50	2.72	16.0	2.3	1.8
C_2H_4	0.41	> 6.1	14.8	1.3	-
H ₂	0.14	2.54	34.5	0.64	0.61
CH ₄	0.46	1.64	17.2	2.5	2.0
CH ₃ OH	0.48	4.08	6.46	1.8	1.5
C ₈ H ₁₈	0.51	4.25	15.1	-	-
C ₃ H ₈	0.51	2.83	15.6	2.0	1.8

Fuel	Minimum ignition energy		
	For	Absolute minimum (10 ⁻⁵ J)	
C_2H_2	3	-	
CO	-	-	
C ₁₀ H ₂₂	-	-	
C ₂ H ₆	42	24	
C ₂ H ₄	9.6	-	
H ₂	2.0	1.8	
CH ₄	33	29	
CH ₃ OH	21.5	14	
C ₈ H ₁₈	_	-	
C ₃ H ₈	30.5	26	

3. Ignition

Most of ignition uses electrical spark (pemantik listrik). Another means is using pilot ignition (flame from very low-flow fuel).

Simplified Ignition Analysis

- Consider Williams' second criterion, applied to a spherical volume of gas, which represents the incipient propagating flame created by a point spark. Using the criterion:
- Find a critical gas-volume radius, R_{crit}, below which flame will not propagate
- Find minimum ignition energy, E_{ign}, to heat critical gas volume from initial state to flame temperature (T_u to T_b).



Figure 8.22. Effect of %fuel on E_{ign}



Figure 8.23. Effect of methane composition on E_{ign}



Table 8.5 Temperature influenceon spark-ignition energy

Fuel	Initial temp (K)	E _{ign} (mJ)
n-heptane	298	14.5
	373	6.7
	444	3.2
Iso-octane	298	27.0
	373	11.0
	444	4.8
n-pentane	243	45.0
	253	14.5

Fuel	Initial temp (K)	E _{ign} (mJ)
n-pentane	298	7.8
	373	4.2
	444	2.3
propane	233	11.7
	243	9.7
	253	8.4
	298	5.5
	331	4.2
	356	3.6
	373	3.5
	477	1.4

Premixed vs diffusion flames



Structure of a diffusion flame (schematic)

2- Laminar diffusion flames

- Seperate feeding of fuel and oxidizer into the combustion chamber
 - Diesel engine
 - Jet engine
- In the combustion chamber:
 - Mixing
 - Subsequently combustion
- Mixing: Convection and diffusion
 - On a molecular level
 → (locally) stoichiometric mixture
- Simple example for a diffusion flame: Candle flame
 - Paraffin vaporizes at the wick
 → diffuses into the surrounding air
- Simultaneously: Air flows towards the flame due to free convection and forms a mixture with the vaporized paraffin





A very difficult flame: the candle flame





• In a first approximation, combustion takes place at locations, where the concentrations of oxygen and fuel prevail in stoichiometric conditions.



Combustion Theory

- The solid fuel is first heated by heat transfer induced by combustion. The liquid fuel reaches the flame by capillarity along the wick and is vaporized.
- Fuel oxidation occurs in thin blue layers (the color corresponds to the spontaneous emission of the CH radical)
- Unburnt carbon particles are formed because the fuel is in excess in the reaction zone. The this soot is the source of the yellow light emission.
- Flow (entrainment of heavy cold fresh air and evacuation of hot light burnt gases) is induced by natural convection

Example : gas lighter

- Fuel enters into the combustion chamber as a round jet
- Forming mixture is ignited
- Example: Flame of a gas lighter
 - Only stable if dimensions are small
 - Dimensions too large: flickering due to influence of gravity
 - Increasing the jet momentum → Reduction of the relative importance of gravity (buoyancy) in favor of momentum forces
 - At high velocities, hydrodynamic instabilities gain increasing importance: laminar-turbulent transition

