COURSE OVERVIEW

DAY 2

Combustion with Flame Propagation

- a. One Dimensional Steady Flow formulation.
- b. Rayleigh and Rankine-Hugoniot equations.
- c. Detonation.
- d. Deflagration. Thermal theory. Flame Speed Dependencies.

Laminar Diffusion Flames

- a. Flame Structure and Mixture Fraction.
- b. Infinitely fast chemistry. Flamelet concept.
- c. 1D Steady Diffusion flames. Strained/Unstrained.
- d. 1D Unsteady Diffusion flames. Strained/Unstrained.
- e. Diluted conditions. Diffusion Ignition processes.



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





FLAME PROPAGATION 1D STEADY FLOW FORMULATION.





FLAME PROPAGATION 1D STEADY FLOW FORMULATION.

in the laboratory frame (the flame propagates to the left at a speed v_0)



in a frame attached to the wave (the flow is steady)



fluid particle velocity $u = v + V_{wave}$

here $V_{\text{wave}} = -v_0$





FLAME PROPAGATION BALANCE EQUATIONS



Giancarlo Sorrentino University "Federico II" of Naples



COURSE OVERVIEW

DAY 2

Combustion with Flame Propagation

- a. One Dimensional Steady Flow formulation.
- b. Rayleigh and Rankine-Hugoniot equations.
- c. Detonation.
- d. Deflagration. Thermal theory. Flame Speed Dependencies.

Laminar Diffusion Flames

- a. Flame Structure and Mixture Fraction.
- b. Infinitely fast chemistry. Flamelet concept.
- c. 1D Steady Diffusion flames. Strained/Unstrained.
- d. 1D Unsteady Diffusion flames. Strained/Unstrained.
- e. Diluted conditions. Diffusion Ignition processes.





FLAME PROPAGATION RAYLEIGH LINES



Giancarlo Sorrentino University "Federico II" of Naples



FLAME PROPAGATION DEFLAGRATION

- Expansion waves, propagate subsonically $(0 < M_0 < 1)$
- The burned gas expands and moves away from the wave front
- In a frame attached to the wave, the downstream flow beyond CJ waves is sonic (M_∞ = 1) for weak deflagrations M_∞ < 1 for strong deflagrations M_∞ > 1
- Wave structure consideration forbids strong deflagrations (there is no structure that connects the burned and unburned states)
- There is a unique solution for the (weak) deflagration giving a definite wave speed for each gas mixture
- Deflagrations are nearly-isobaric ($p \approx \text{const.}$) such that $\rho \sim 1/T$ and propagate slowly $v_0 \sim 10 100 \text{ cm/s}$, producing heat



FLAME PROPAGATION DETONATION

- Compression waves, propagate supersonically $(1 < M_0 < \infty)$
- · The wave retards the burned gas that compresses behind the wave front
- In a frame attached to the wave, the downstream flow beyond CJ waves is sonic (M_∞ = 1) for weak detonations M_∞ > 1 for strong detonations M_∞ < 1
- A strong detonation can be produced by driving a piston at an appropriate speed
- There is only one wave speed at which a weak detonation can propagate (weak detonations are seldom observed)
- Self-sustained detonations are CJ detonations
- Detonations are rapid (v₀ ~ 3000 m/s) and violent (p_∞/p₀ ~ 20), with a significant increase in temperature (T_∞/T₀ ~ 10)





FLAME PROPAGATION RANKINE-HUGONIOT

FROM BALANCE EQUATIONS:

$$h_2^s - h_1^s = \frac{(p_2 - p_1)}{2} \left(\frac{1}{\rho_2} + \frac{1}{\rho_1}\right) + \Delta h^o$$

HP: -IDEAL GAS - C_P= COST

$$\frac{\gamma}{\gamma-1}\left(\frac{p_2}{\rho_2}-\frac{p_1}{\rho_1}\right) = \frac{(p_2-p_1)}{2}\left(\frac{1}{\rho_2}+\frac{1}{\rho_1}\right) + \Delta h^o$$

 $h^{s} = c_{\rho}T = \frac{c_{\rho}}{R}\frac{\rho}{\rho} = \frac{\gamma}{\gamma - 1}\frac{\rho}{\rho}$

PRESSURE RATIO







FLAME PROPAGATION RANKINE-HUGONIOT CURVES



FLAME PROPAGATION

Giancarlo Sorrentino University "Federico II" of Naples

FLAME PROPAGATION CLASSIFICATION

| Strong Detonation | $p_2 > p_{CJ} > p_1$ | | |
|----------------------------|-----------------------|--|--|
| Chapman-Jouguet Detonation | $p_2 = p_{CJ} > p_1$ | | |
| Weak Detonation | $p_{CJ} > p_2 > p_1$ | | |
| Weak Deflagration | $p_1 > p_2 > p_{lim}$ | | |
| Limit Deflagration | $p_1 > p_{im} = p_2$ | | |
| Strong Deflagration | $p_1 > p_{im} > p_2$ | | |

COURSE OVERVIEW

DAY 2

Combustion with Flame Propagation

- a. One Dimensional Steady Flow formulation.
- b. Rayleigh and Rankine-Hugoniot equations.
- c. Detonation.
- d. Deflagration. Thermal theory. Flame Speed Dependencies.

Laminar Diffusion Flames

- a. Flame Structure and Mixture Fraction.
- b. Infinitely fast chemistry. Flamelet concept.
- c. 1D Steady Diffusion flames. Strained/Unstrained.
- d. 1D Unsteady Diffusion flames. Strained/Unstrained.
- e. Diluted conditions. Diffusion Ignition processes.

FLAME PROPAGATION CLASSIFICATION

Giancarlo Sorrentino University "Federico II" of Naples

DETONATION

Detonation is a combustion process in which there is a compression of the gaseous mixture from the inlet condition to products.

In the case of stationary detonation and due to the constraints imposed by the conservation of mass, momentum and total enthalpy, gases also undergo a density increasing and deceleration.

The detonation is defined as strong or weak depending on whether the pressure is greater or less than that of "Chapman-Jouguet (C-J).

The latter is defined as the solution obtained when the Rayleigh line is tangent to the Rankine-Hugoniot curve and takes its name from the authors (Chapman D.L, 1899; Jouguet E., 1906).

DETONATION C-J CONDITION

Rankine-Hugoniot and Rayleigh curves admit a single solution in the conditions of Chapman-Jouguet (C-J), i.e. where the two curves are tangent to each other. The generic tangent to the curve of Rankine Hugoniot is given by the derivative of the pressure (p2) in relation to the specific volume (1/p2). This can be obtained, in turn, by deriving, with respect to 1/p2 both the members of the Rankine Hugoniot.

$$\frac{\gamma}{\gamma - 1} \frac{1}{\rho_2} \frac{dp_2}{d(1/\rho_2)} + \frac{\gamma}{\gamma - 1} p_2 = \frac{1}{2} \frac{dp_2}{d(1/\rho_2)} \left(\frac{1}{\rho_2} + \frac{1}{\rho_1}\right) + \frac{p_2 - p_1}{2}$$

DETONATION C-J CONDITION

$$\begin{split} \frac{\gamma}{\gamma - 1} \frac{1}{\rho_2} \frac{dp_2}{d(1/\rho_2)} + \frac{\gamma}{\gamma - 1} p_2 &= \frac{1}{2} \frac{dp_2}{d(1/\rho_2)} \left(\frac{1}{\rho_2} + \frac{1}{\rho_1} \right) + \frac{p_2 - p_1}{2} \\ \frac{\gamma}{\gamma - 1} \frac{1}{\rho_2} \left(-\dot{\mathcal{M}}^2 \right) + \frac{\gamma}{\gamma - 1} p_2 &= \frac{1}{2} \left(-\dot{\mathcal{M}}^2 \right) \left(\frac{1}{\rho_2} + \frac{1}{\rho_1} \right) + \frac{1}{2} \left(-\dot{\mathcal{M}}^2 \right) \left(\frac{1}{\rho_2} - \frac{1}{\rho_1} \right) \\ &- \dot{\mathcal{M}}^2 \left(\frac{\gamma}{\gamma - 1} \frac{1}{\rho_2} - \frac{1}{\rho_2} \right) = -\frac{\gamma}{\gamma - 1} p_2 \\ u_2^2 &= \gamma \frac{p_2}{\rho_2} = \gamma R T_2 \\ u_2 \Big|_{CJ} &= \alpha_2 \Big|_{CJ} \end{split}$$

DETONATION

$$\frac{\gamma+1}{\gamma} \ge \frac{\rho_2}{\rho_1} \ge 1$$

$$\frac{p_2}{p_1} = \frac{\rho_2}{\rho_1} \frac{T_2}{T_1}$$

$$u_{2_{CJ}} = \alpha_{2_{CJ}} = O(1000 \text{ms}^{-1})$$

$$u_1 \Big|_{CJ} = \frac{\rho_2}{\rho_1} u_2 \Big|_{CJ} = 2 * O(1000 \text{ms}^{-1}) = O(2000 \text{ms}^{-1})$$

DETONATION

| H ₂ /O2 100 kPa 298 K | H2 % | D-CJ m/s | D-CJ % |
|--|--------|----------|--------|
| | 66 | 2818 | 1.6 |
| | 80 | 3408 | 2 |
| | 85 | 3638 | 5 |
| | 87 | 3720 | 6 |
| | 88 | 3755 | 7 |
| | | | |
| H2/CO/O2/Ar 33/30/16.7/50 298 K | p, kPa | D-CJ m/s | D-CJ % |
| | 33.3 | 1629 | 3.7 |
| | 26.7 | 1623 | 3.5 |
| | 20.1 | 1615 | 5.4 |
| | 13.3 | 1603 | 7.3 |
| | | | |

DI C Ma PI

The ZND structure

Zel'dovich (1940), von Neuman (1942), Doring (1944)

inert shock followed by a fast deflagration

Giancarlo Sorrentino University "Federico II" of Naples

The lowest possible Rayleigh line is the one tangent to the complete-reaction Hugoniot (i.e., corresponding to $\lambda = 1$). The final state in this case is the Chapman-Jouguet (CJ) state. The corresponding detonation speed D_{CJ} is the minimum speed consistent with the conservation laws.

The ZND structure is not possible for weak detonations

COURSE OVERVIEW

DAY 2

Combustion with Flame Propagation

- a. One Dimensional Steady Flow formulation.
- b. Rayleigh and Rankine-Hugoniot equations.
- c. Detonation.
- d. Deflagration. Thermal theory. Flame Speed Dependencies.

Laminar Diffusion Flames

- a. Flame Structure and Mixture Fraction.
- b. Infinitely fast chemistry. Flamelet concept.
- c. 1D Steady Diffusion flames. Strained/Unstrained.
- d. 1D Unsteady Diffusion flames. Strained/Unstrained.
- e. Diluted conditions. Diffusion Ignition processes.

DEFLAGRATION

A propagation process, in which the release of energy generates an expansion (lowering of density and pressure) in the region occupied by the products of the oxidation reaction, is called **deflagration**.

The lowering of the pressure is almost always a negligible fraction of the average pressure detectable in the whole region affected by the combustion process. Therefore, the process is considered almost isobaric. The expansion of the part of the mixture in which the combustion took

place generates the velocity increase.

The region of the space in which the combustion process propagates during deflagration is usually referred to as the "flame front" or "combustion wave". The terms "deflagration" and "laminar premixed flame" are used in practice in the same scientific sense, although the second (flame) is generally associated with phenomena of light emission that extend its meaning in common use.

DEFLAGRATION

 $\rho_2 < \rho_1$

DEFLAGRATION

Frame moving with the flame

The one-dimensional field is divided in 3 zones in series:

I) Region governed by convection and diffusion

2) Region governed by the convection and production of sensible enthalpy up to T_F

3) Region governed by the convection and enthalpy production up to Tad

Balance of sensible enthalpy

Balance of chemical enthalpy

$$\frac{\partial \rho h^{s}}{\partial t} + \underline{\nabla} \rho \underline{\vee} h^{s} - \underline{\nabla} (\rho \alpha \underline{\nabla} h^{s}) = -\sum \dot{\rho}_{i} h_{i}^{o}$$
$$\frac{\partial \rho h^{o}}{\partial t} + \underline{\nabla} \rho \underline{\vee} h^{o} - \underline{\nabla} J_{h^{o}} = \sum \dot{\rho}_{i} h_{i}^{o}$$

Hp:

- <u>ID</u>

- <u>Stationary</u>

$$\frac{d(\rho u h^s)}{dx} - \frac{d}{dx} \left(\rho \frac{d}{dx} h^s \right) = 0$$

$$\frac{d(\rho u h^o)}{dx} = \sum \dot{\rho}_i h_i^o$$

Balance of Sensible Enthalpy in l_{DF}

Balance of Chemical Enthalpy l_F

Cp=constant

$$d\left[\rho uT - \rho \alpha \frac{dT}{dx}\right] = 0$$

integrating between the undisturbed condition (subscript 0) and the condition of ignition (subscript i), also considering that the convective flow of mass is a constant, is obtained

$$\rho u(T_i - T_o) - \rho_i \alpha_i \left(\frac{dT}{dx}\right)_i = 0$$

 $\left(\frac{dT}{dx}\right) = \frac{T_F - T_i}{I_F}$

 $U_i = V_F$

Hp:

- Linear Temperature gradient in the flame region
- Convective flux evaluated in the Ignition point
- Flame Speed is defined as:

$$v_F I_F = \alpha_i \frac{T_F - T_i}{T_i - T_o}$$

The Laminar Flame Speed V_F is the gas velocity in the ignition point

Relation between flame speed and flame thickness

$$\mathbf{v}_F \mathbf{I}_F = \alpha_i \frac{T_F - T_i}{T_i - T_o}$$

Burning velocity

$$u_{o} = \frac{\rho_{i}}{\rho_{o}} v_{F}$$

Integrating twice the balance of sensible enthalpy in the region controlled by the diffusion

$$\mathbf{v}_{F}I_{DF} = \alpha_{i} \ln\left(\frac{T_{i} - T_{o}}{T - T_{o}}\right)$$

Flame speed estimation

$$\mathbf{v}_F \mathbf{I}_F = \alpha_i \frac{T_F - T_i}{T_i - T_o}$$

Integrating the balance of chemical enthalpy in the flame region

$$\rho_i u_i \left[h_F^o - h_i^o \right] = \int_{x_i}^{x_F} \sum \left(\dot{\rho}_i h_i^o \right) dx$$

we can define a conversion degree

$$\varepsilon(x) = \frac{\sum \dot{\rho}_i h_i^o}{\rho_i [h_F^o - h_i^o]}$$
$$\mathbf{v}_F = \int_i^F \varepsilon(x) \, dx = \overline{\varepsilon} \, I_F$$

$$\varepsilon(\mathbf{x}):$$

 $\overline{\varepsilon} \propto \exp\left(-\frac{1}{T}\right) p^{n-1}$

$$v_F = \sqrt{\alpha_i \frac{T_F - T_i}{T_i - T_o} \varepsilon}$$

Deflagration/dependencies

$$\mathbf{v}_F I_F = \alpha_i \frac{T_F - T_i}{T_i - T_o} \qquad \mathbf{v}_F I_{DF} = \alpha_i \ln\left(\frac{T_i - T_o}{T - T_o}\right)$$

$$v_F = \sqrt{\alpha_i \frac{T_F - T_i}{T_i - T_o}} \varepsilon$$

Laminar flame speed depends on various parameters such as ambient temperature, air/fuel ratio, fuel nature and pressure

Effect of ambient temperature

effect of fuel/air ratio

flammability limits

Definition:

- Limiting composition for (premixed) flame propagation
 - ⇒ a limit at which heat generation cannot keep up with (heat) loss
- Some amount of heat or radical loss is essential
- Ideally, it is believed to be a fundamental quantity for a given fuel/oxidizer mixture.

flammability limits

Empirical Limits

- LFL (lean) and UFL (rich)
- Depends on experimental configuration
- US Bureau of Mines
 51mm x 1.5m tube
 Upward (more conservative)
 & downward propagation
- Temperature increase
 ⇒ both LFL/UFL widens
- Pressure increase
 - \Rightarrow LFL: narrows
 - ⇒ UFL: narrows for H₂ widens for other hydrocarbons

| Fuel | Lean Limit | Rich Limit | | |
|-------------------------------|-------------|-------------|--|--|
| H ₂ | 4.00 (0.10) | 75.0 (7.14) | | |
| со | 12.5 (0.34) | 74.0 (6.8) | | |
| NH ₃ | 15.0 (0.63) | 28.0 (1.4) | | |
| CH₄ | 5.0 (0.50) | 14.9 (1.67) | | |
| C_2H_6 | 3.0 (0.52) | 12.4 (2.4) | | |
| C ₃ H ₈ | 2.1 (0.56) | 9.5 (2.7) | | |
| C_4H_{10} | 1.8 (0.57) | 8.4 (2.8) | | |
| C ₂ H ₄ | 2.7 (0.40) | 36.0 (8.0) | | |
| C_2H_2 | 2.5 (0.31) | 100.0 (∞) | | |
| C ₆ H ₆ | 1.3 (0.56) | 7.9 (3.7) | | |
| CH₃OH | 6.7 (0.51) | 36.0 (4.0) | | |
| C₂H₅OH | 3.3 (0.41) | 19.0 (2.8) | | |

Flammability limits at 1atm, in mole % and (\u00ft): Zabetakis, US Dept. of Mines Bulletin 627 (1965).

flammability limits

Le Chatelier's Rule (Empirical Rule for Mixture)

For a mixture of N components:

$$(LFL)_{mixture} = \left[\sum_{i=1}^{N} \frac{X_i}{(LFL)_i}\right]^{-1}$$

e.g. for 50% hydrogen and 50% CO:

$$(LFL)_{mixture} = \left[\frac{0.5}{4} + \frac{0.5}{12.5}\right]^{-1} = 6.1\%$$

where X_i : mole fraction of the *i*th component

The rule can be extended for a fuel with dilution:

$$\left(LFL\right)_{dilution} = \left[\frac{X_F}{\left(LFL\right)_F} + \frac{X_I}{\left(LFL\right)_I}\right]^{-1} = \frac{\left(LFL\right)_F}{X_F}$$

since $(LFL)_I \rightarrow \infty$ For a mixture of fuels and dilution:

$$(LFL)_{mixture, dilution} = \frac{(LFL)_{mixture}}{X_{mixture}}$$

Inert effect

% of Inert added to the mixture

Fuel nature effects

Effect of the Pressure

It is observed experimentally that u_0 does not depend on the pressure for many fuels so it can be assumed that the overall order n of the reaction is about 2.

single-step reaction rate parameters

(best agreement between experimental/computational flammability limits)

$$\omega = \mathcal{B} \exp - (E_a / \mathcal{R}T) \ [\text{Fuel}]^a [\text{Oxidizer}]^b$$

Single-step reaction rate parameters giving best agreement between experimental flammability limits (ϕ_L ' and ϕ_R) and computed flammability limits (ϕ_L and ϕ_R). Units are cm-sec-mole-kcal-Kelvins

| Fuel | A | Ea | a | b | φι.' | ϕ_L | φ <i>R</i> ′ | φ _R |
|----------------------------------|------------------------|------|------|------|------|----------|--------------|----------------|
| CH4 | 1.3 × 10 ⁸ | 48.4 | -0.3 | 1.3 | 0.5 | 0.5 | 1.6 | 1.6 |
| CH4 | 8.3×10^{5} | 30.0 | -0.3 | 1.3 | 0.5 | 0.5 | 1.6 | 1.6 |
| C ₂ H ₆ | 1.1×10^{12} | 30.0 | 0.1 | 1.65 | 0.5 | 0.5 | 2.7 | 3.1 |
| C ₃ H ₈ | 8.6×10^{11} | 30.0 | 0.1 | 1.65 | 0.5 | 0.5 | 2.8 | 3.2 |
| C4H10 | 7.4 × 1011 | 30.0 | 0.15 | 1.6 | 0.5 | 0.5 | 3.3 | 3.4 |
| C5H12 | 6.4×10^{11} | 30.0 | 0.25 | 1.5 | 0.5 | 0.5 | 3.6 | 3.7 |
| C6H14 | 5.7 × 1011 | 30.0 | 0.25 | 1.5 | 0.5 | 0.5 | 4.0 | 4.1 |
| C7H16 | 5.1 × 10 ¹¹ | 30.0 | 0.25 | 1.5 | 0.5 | 0.5 | 4.5 | 4.5 |
| C ₈ H ₁₈ | 4.6×10^{11} | 30.0 | 0.25 | 1.5 | 0.5 | 0.5 | 4.3 | 4.5 |
| C ₈ H ₁₈ | 7.2×10^{12} | 40.0 | 0.25 | 1.5 | 0.5 | 0.5 | 4.3 | 4.5 |
| C9H20 | 4.2×10^{11} | 30.0 | 0.25 | 1.5 | 0.5 | 0.5 | 4.3 | 4.5 |
| C10H22 | 3.8×10^{11} | 30.0 | 0.25 | 1.5 | 0.5 | 0.5 | 4.2 | 4.5 |
| CH ₃ OH | 3.2×10^{12} | 30.0 | 0.25 | 1.5 | 0.5 | 0.5 | 4.1 | 4.0 |
| C ₂ H ₅ OH | 1.5×10^{12} | 30.0 | 0.15 | 1.6 | 0.5 | 0.5 | 3.4 | 3.6 |
| CeHe | 2.0×10^{11} | 30.0 | -0.1 | 1.85 | 0.5 | 0.5 | 3.4 | 3.6 |
| C ₇ H ₈ | 1.6×10^{11} | 30.0 | -0.1 | 1.85 | 0.5 | 0.5 | 3.2 | 3.5 |
| C ₂ H ₄ | 2.0×10^{12} | 30.0 | 0.1 | 1.65 | 0.4 | 0.4 | 6.7 | 6.5 |
| C ₂ H ₆ | 4.2×10^{11} | 30.0 | -0.1 | 1.85 | 0.5 | 0.5 | 2.8 | 3.0 |
| C_2H_2 | 6.5×10^{12} | 30.0 | 0.5 | 1.25 | 0.3 | 0.3 | >10.0 | >10.0 |

Westbrook & Dryer, CST 1981

 $E_a \approx 30 - 50 \text{ kcal/mole}\cdot \text{K}$ $\mathcal{R} = 1.987 \text{ cal/g} \cdot \text{mol K}$

$$\Rightarrow \quad E_a/\mathcal{R} \approx 18,000 \,\mathrm{K}$$

Zel'dovich number

 $\beta \sim 10~$ for hydrocarbon-air flames

$$\beta_0 = \frac{\beta T_a^2}{T_a - 1} \quad \Rightarrow \qquad \omega = D \rho^n Y_F^{n_F} Y_O^{n_O} \exp\left[\frac{\beta T_a}{T_a - 1} \left(\frac{T - T_a}{T}\right)\right]$$

Reaction is confined within a thin layer of $\delta_R \sim \delta_T / \beta$

COURSE OVERVIEW

DAY 2

Combustion with Flame Propagation

- a. One Dimensional Steady Flow formulation.
- b. Rayleigh and Rankine-Hugoniot equations.
- c. Detonation.
- d. Deflagration. Thermal theory. Flame Speed Dependencies.

Laminar Diffusion Flames

- a. Flame Structure and Mixture Fraction.
- b. Infinitely fast chemistry. Flamelet concept.
- c. 1D Steady Diffusion flames. Strained/Unstrained.
- d. 1D Unsteady Diffusion flames. Strained/Unstrained.
- e. Diluted conditions. Diffusion Ignition processes.

