4A13: Combustion and Engines

Summarized from N. Swaminathan and S. Hochgreb lectures

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Last updated: April 25, 2022

Contents

1 Chapter 1: Basics

Combustion: Chemical reaction between fuel and oxidiser involving significant release of heat.

1.1 Basic concepts

- Equivalence ratio

$$\phi = \frac{m_{fuel}/m_{air}}{(m_{fuel}/m_{air})_{st}} = \frac{V_{fuel}/V_{air}}{(V_{fuel}/V_{air})_{st}}$$

- Air-fuel ratio

$$AFR = \frac{1}{\phi}AFR_{st}$$

$$AFR_{st} = \frac{m_{air}}{m_{fuel}}$$

$$AFR_{st,vol} = \frac{n_{air}}{n_{fuel}}$$

(directly from balanced reaction equation)

1.2 Combustion reaction

$$C_xH_y + \frac{a}{\phi}(O_2 + \frac{0.79}{0.21}N_2) \longrightarrow a_1CO_2 + a_2CO + a_3H_2O + a_4H_2 + a_5O_2 + \frac{a}{\phi}\frac{0.79}{0.21}N_2$$
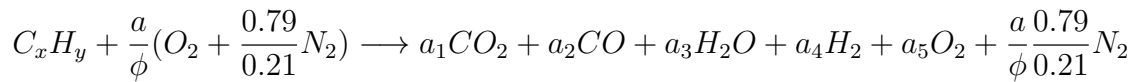
- Case 1: $\phi \leq 1$

$$a_2 = a_4 = 0$$

$$a_1 = x$$

$$a_3 = \frac{y}{4}$$

$$a_5 = \frac{a(1-\phi)}{\phi}$$

- Case 2: $\phi > 1$

$$a_2 \neq 0$$

$$a_4 \neq 0$$

  – Cannot calculate final product composition by atom conservation. See Ch 3.

1.3 Mixture properties

- Molar fraction
$$X_k = \frac{n_k}{n_{tot}}$$

- Mass fraction
$$Y_k = \frac{m_k}{m_{tot}}$$

- Total molecular weight
$$Y_k = \frac{M_k}{M_{tot}} X_k$$

$$M_{tot} = \sum_k X_k M_k = \frac{1}{\sum_k \frac{Y_k}{M_k}}$$

- Concentration
$$C_k = \frac{X_k n_{tot}}{V} = X_k \frac{P}{R^0 T} = Y_k \frac{\rho}{M_k}$$

- Density
$$\rho = \sum_k X_k \rho_k$$

(Can be approximated to ρ_{air} due to abundance of N_2.)

- Pressure
$$P_k = X_k P$$

- Enthalpy *(kJ/kmol or kJ/kg)*
$$h = \sum_k Y_k h_k$$

$$\overline{h} = \sum_k X_k \overline{h_k}$$

$$h_k = \frac{\overline{h_k}}{M_k}$$

$$h = \frac{\overline{h}}{M_{tot}}$$

(Molar quantities are denoted by overbars)

1.4 Heat of combustion and adiabatic flame temperature

Assumptions:

- Constant c_p.

- Constant pressure.
$$Y_{fuel} Q = c_p (T_f - T_i)$$

$$(c_p = c_p(T = \tfrac{T_i + T_f}{2}) \text{ for better accuracy})$$

1.5   1D balance equations

- Species

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial \rho(U Y_k)}{\partial x} = \frac{\partial}{\partial x}(\rho D \frac{\partial Y_k}{\partial x}) + \dot{w}_k$$

- Energy ($c_p = cst$, $Le = 1$)

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p U \frac{\partial T}{\partial x} = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x}(\lambda \frac{\partial T}{\partial x}) - Q\dot{w}_{fuel}$$
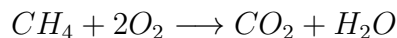
1.6   Worked problems

1. Molar fractions aren't conserved in chemical reactions (mass fractions are).

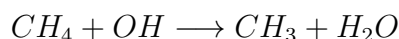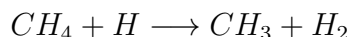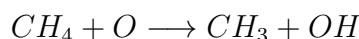2. Dry mixture doesn't contain water ($X_{H_2O} = 0$).

2 Chapter 2: Kinetics and chemistry

2.1 Global and elemental reactions

- **Global reactions**
$$CH_4 + 2O_2 \longrightarrow CO_2 + H_2O$$

In reality, this is impossible because the reactions involves too many bonds to break. We talk about **elementary reactions** instead:

$$CH_4 + O \longrightarrow CH_3 + OH$$

$$CH_4 + H \longrightarrow CH_3 + H_2$$
$$CH_4 + OH \longrightarrow CH_3 + H_2O$$

- Hundreds or thousands of elemental reactions.

- **Radicals** (unstable and very reactive molecules, i.e: OH, H, O, CH_3, HO_2, NO, anything that isn't H_20 or CO_2) appear.

- **Chemical mechanism:** Series of elemental reactions.

2.2 Law of mass action

- Only valid for elemental reactions:

$$a_1 R_1 + a_2 R_2 \longrightarrow b_1 P_1 + b_2 P_2$$
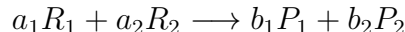
- **Law of mass action**
$$\omega = k[R_1]^{a_1}[R_2]^{a_2}$$

where ω is the reaction rate and k is the reaction rate constant.

  - ω is independent of products.

- **Arrhenius law** – <u>empirical</u>

$$k = Ae^{-\frac{E_{act}}{R^0 T}} = Ae^{-\frac{T_{act}}{T}}$$

where A is the pre-exponential factor, E_{act} is the activation energy, R^0 is the gas constant, and T is the *temperature of the <u>vessel</u>*.

  - k is independent of product concentrations.
  - When T increases, k increases, and the reaction rate increases with temperature.

2.3 Reaction mechanisms

- Net consumption of product/reactant can be obtained by summing multiple elementary reactions:
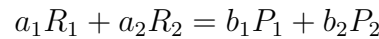 *Example:*
  $$\frac{d[CH_4]}{dt} = -k_1[CH_4][O] - k_2[CH_4][H] - k_3[CH_4][OH]$$

- Backward-forward reactions:

  $$a_1 R_1 + a_2 R_2 = b_1 P_1 + b_2 P_2$$

  $$\frac{dR_1}{dt} = -k_f[R_1]^{a_1}[R_2]^{a_2} + k_b[P_1]^{b_1}[P_2]^{b_2}$$

- **Reaction rate in species balance equation**
  Example: Zeldovich mechanism

  $$N_2 + O = NO + N$$

  $$N + O_2 = NO + O$$
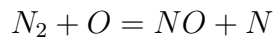
  Reaction rate $\omega \, (kmol/m^3 s)$

  $$\hat{w}_{NO} = k_{1f}[N_2][O] - k_{1b}[NO][N] + k_{2f}[N][O_2] - k_{2b}[NO][O]$$

  Reaction rate in species balance $\dot{w} \, (kg/m^3 s)$

  $$\dot{w}_{NO} = \hat{w}_{NO}(a_{NO} M(NO))$$

  where a_{N0} is the stoichiometric coefficient of NO (in this case, $a_{NO} = 1$).

2.4 Types of elementary reactions

- **Order** *or* **molecularity**
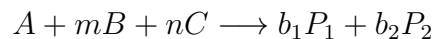
  $$A + mB + nC \longrightarrow b_1 P_1 + b_2 P_2$$
  $$O = 1 + m + n$$

  - 1st order: very unlikely to happen spontaneously (usually need two molecules to collide)
  - 2nd order: most common.
  - 3rd order: unlikely, but can happen in *radical recombination reactions.*

- **Chain reactions**

  1. Chain-initiating (no radical in reactants)

  $$H_2 + M \longrightarrow H + H + M$$

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2. Chain-branching (radicals on each side but more on the products' side)

$$H + O_2 \longrightarrow OH + O$$

3. Chain-propagating (same number of radicals in both sides)

$$HO_2 + H \longrightarrow OH + OH$$

4. Chain-terminating (no radicals in products)

$$H + OH + M \longrightarrow H_2O + M$$
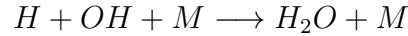
2.5   Simplified chemical mechanisms

- **One-step combustion**

$$C_xH_y + \frac{a}{\phi}(O_2 + \frac{0.79}{0.21}N_2) \longrightarrow a_1CO_2 + a_3H_2O + a_4O_2 + \frac{a}{\phi}\frac{0.79}{0.21}N_2$$

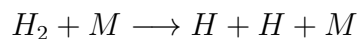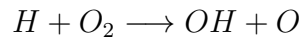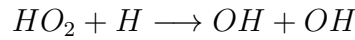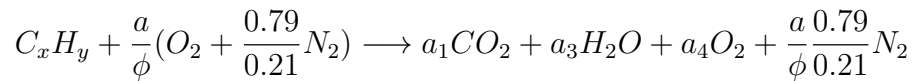$$\frac{d[C_xH_y]}{dt} = -A_G e^{-\frac{T_{act}}{T}}[C_xH_y]^p[O_2]^q$$

p and q have nothing to do with stoichiometric coefficients.
In this course, we use $p = q = 1$.

- **Systematically reduced combustion**

  1. **Steady-state approximation**
     Species A is in steady-state if:
     $$\frac{dA}{dt} \approx 0$$
     Example: Zeldovich mechanism: N radical is consumed as soon as it is produced:
     $$\frac{dN}{dt} \approx 0$$
     Plug this in net backward-forward reaction rate, solve for [N] as a function of other species.
     Plug in net reaction rate of NO and neglect backward reactions:
     $$\frac{d[NO]}{dt} = 2k_{1f}[N_2][O]$$

  2. **Partial equilibrium assumption**
     Forward and backward rates are equal.
     $$O2 = 2O$$
     $$[O] = \sqrt{\frac{k_{2f}}{k_{2b}}} \ [O]^{1/2}$$
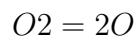
- **Reduced NO mechanism**

$$N_2 + O_2 \longrightarrow 2NO$$
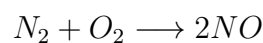
$$\frac{d[NO]}{dt} = 2k_{1f}[N_2]\sqrt{\frac{k_{2f}}{k_{2b}}} \ [O]^{1/2}$$

2.6 Typical combustion sequence

1. Breakdown of fuel into smaller hydrocarbons. These could be stable species (not necessarily radicals).

2. All carbon results in CO and all the hydrogen results in H_2.

3. Final oxidation of CO and H_2 into CO_2 and H_2O. This is where the largest part of the heat release happens. The elementary reactions involved are:

$$CO + OH \longrightarrow CO_2 + H$$

$$H_2 + OH \longrightarrow H_2O + H$$
$$H + OH + M \longrightarrow H_2O + M$$
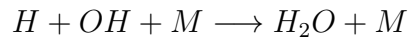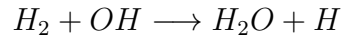
2.7 Worked problems

1. Arrhenius law with T_{act}. Exponential decay of species concentration à la nuclear fission decay. Integral with log. High temperature or high pressure results in quicker reactions.

2. Didn't obtain the same values here. Molar fractions are obtained from air composition (i.e: 0.21 and 0.79). Other than that, simple plug and compute.

3   Chapter 3: Dissociation

- The adiabatic flame temperature calculated in chapter 1 (under the assumption of chemical equilibrium) is, in reality, overestimated because part of the heat is used to initiate endothermic dissociation reactions.

- A more accurate estimate of combustion temperature has to take dissociation reactions into consideration.

- This is how we are able to estimate the adiabatic flame temperature of incomplete combustion reactions (i.e: typically $\phi > 1$).

3.1   Definition

- **Dissociation :** decomposition of combustion <u>products</u> at high temperatures.

- This may lead to other dissociations.

- Dissociation mostly affects CO_2 and H_2O at typical combustion temperatures.

3.2   Chemical equilibrium

$$CO + \frac{1}{2}O_2 = CO_2$$
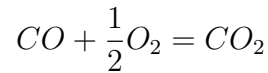
- This reaction usually goes from lhs to rhs but eventually reaches a point of equilibrium when the forward and backward reactions are in perfect balance. At equilibrium, the reaction rate is null:

$$w_i = 0$$

- The equilibrium will be the one that gives the maximum entropy of the whole mixture:

$$S = S_{max}$$

$$dS = 0$$

- **Equilibrium constants**

  - **Gibbs free energy:**

$$G = H - TS$$

$$G_{mix} = \sum_i n_i \overline{g_i} = \sum_i n_i(\overline{g}_i^0 + R^0 T ln(P_i/P^0))$$

At equilibrium, $P = cst$ and $T = cst$:

$$dG = 0$$

We define the equilibrium constant as a criteria for equilibrium:

$$K_p = \frac{\prod_{products}(P_i/P^0)^{b_i}}{\prod_{reactants}(P_i/P^0)^{a_i}}$$

where P_i is the partial pressure, P^0 is the standard state pressure (usually 1 bar or 1 atm), b_i and a_i the stoichiometric factors from the equilibrium reactions (check Thermofluids databook).

– **Reaction rate :** If a reaction is in equilibrium, then:

$$\omega_{forward} = \omega_{backward}$$

$$\frac{k_f}{k_b} = f(K_p)$$

• **Le Châtelier's principle :** When a change of pressure or temperature happens, the equilibrium point will shift towards the reactants or the products to minimise the change.

– When **pressure** increases = less dissociation.

– When **temperature** increases = more dissociation.

Reaction possible or impossible?

- II law of thermodynamics => $ds > 0$ for a natural process
- from thermodynamics, Gibbs free energy **dg = dh - Tds**
- for a natural process $dg < 0$; $dg = 0$ at equilibrium

No	h	s	g	Remark
1	-	+	-	Possible at all T (also exothermic)
2	-	-	-/+	Possible at low T; impossible at high T
3	+	+	-/+	Possible at high T; impossible at low T
4	+	-	+	Impossible at all T

$N_2 + 0.5\,O_2 \longrightarrow N_2O$ is this possible at T=300K & P=1.0 atm ?

$H_2O(l) \longrightarrow H_2O$ at what T does this reaction occur for P = 1.0 atm?

3.3   Worked examples

Steps:

1. Write chemical reaction equation.

2. System of equations with stoichiometric factors as unknowns.

3. Find the equilibrium reaction of the <u>products</u> of the reaction.

4. Find an additional equation with K_p using the stoichiometric coefficients of the <u>products</u> in the original equation:

$$K_p = f(b_i)$$

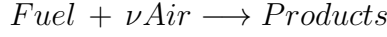where b_i are the stoichiometric factors of products.

5. Solve system of equations for stoichiometric factors.

6. Calculate species composition in original equation.

4 Chapter 4: Autoignition

4.1 Introduction

4.1.1 Conserved scalar

We assume a one-step reaction such that:

$$Fuel + \nu Air \longrightarrow Products$$

The reaction rate in the species balance equation is:

$$\dot{w}_{fuel} = -Aexp(-\frac{E_a}{R^0 T_0})(\frac{M_{fuel}}{M_{fuel} M_{ox}}\rho^2 Y_f Y_{ox})$$

We combine the species and heat balance equations:

- Species

$$Q * [\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial \rho(U Y_k)}{\partial x} = \frac{\partial}{\partial x}(\rho D \frac{\partial Y_k}{\partial x}) + \dot{w}_k]$$

- Energy $(c_p = cst, Le = 1)$

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p U \frac{\partial T}{\partial x} = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x}(\lambda \frac{\partial T}{\partial x}) - Q\dot{w}_{fuel}$$

We obtain a balance equation for the scalar

$$Z = QY_k + c_p T$$

By conservation of this scalar, we obtain:

$$Y_f = Y_{f,0} - c_p \frac{T - T_0}{Q}$$

$$Y_{ox} = Y_{ox,0} - S.c_p \frac{T - T_0}{Q}$$

where $S = \frac{\nu M_{ox}}{M_f}$.

4.1.2 Maximum temperature

We obtain, similar to Chapter 1, the following relation:

$$T_f = \frac{Y_f Q}{c_p} + T_0$$

4.1.3 Reaction rate

This simple thermochemical models allows us to define the reaction rate as a function of the temperature only:

$$\dot{w}_{fuel} = C.f(T)$$
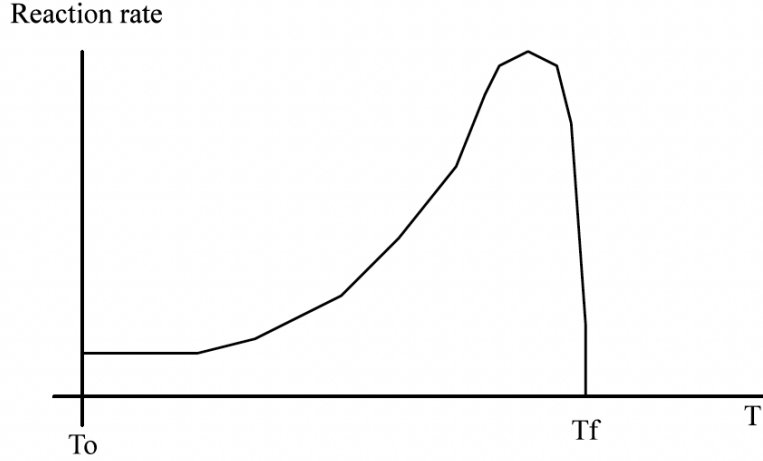
Figure 4-2. Dependence of the reaction rate on the temperature for an adiabatic system obeying Eqs. (4.1), (4.5) and (4.6). T_0 is the initial temperature and T_f the adiabatic flame temperature.

4.2 Autoignition without heat losses

– Assumptions

- Constant pressure, adiabatic, closed vessel.

- Ignition stage (no combustion yet but chemical reactions happen).

- No diffusion.

- No convection.

During the ignition stage, we assume temperature is very low:

$$x = \frac{\nabla T}{T_0} \approx small$$

So, we perform a "trick":

$$\frac{1}{1+x} \approx 1 - x$$

The ignition delay time is the difference between t_0 and when the temperature crosses a given threshold (can be the time when the temperature becomes infinite $T \sim \infty$).
We define the ignition delay time by:

$$\tau_{ign} = (\frac{Q}{c_p} \frac{M_f}{M_f + M_{ox}} \rho_0 A Y_{fu,0} Y_{ox,0})^{-1} \frac{R^0 T_0^2}{E_a} exp(\frac{E}{R^0 T_0})$$

– Effect of:

- **Initial temperature:** $T \uparrow \Rightarrow \tau_{ign} \downarrow$
  By differentiation:

$$\frac{d\tau_{ign}}{T_0} = \frac{\tau_{ign}}{T_0}(2 - \frac{E}{R^0 T_0})$$

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- **Pressure:** $P \uparrow \Rightarrow \tau_{ign} \downarrow$
  Appears through the density term ρ_0

- **Mass fractions of reactants:** Y_f, $Y_{ox} \uparrow \Rightarrow \tau_{ign} \downarrow$

4.3 Autoignition with heat losses

– Same hypotheses as before except the vessel is no longer adiabatic and the pressure is no longer constant (?)
We have:
$$\frac{\partial T}{\partial t} = \frac{1}{\rho c_v} Q \dot{w}_{fuel} - \frac{A}{\rho c_v V} h(T - T_0) = G - L$$
where h is the heat transfer coefficient (not enthalpy), G is the rate of heat release due to chemical reaction (nonlinear with T), and L is a heat loss term (L varies linearly with T). – **Cases**

1. $G > L$: Ignition.

2. $G = L$: Stable or unstable (depending on location, check graphs).

3. $G < L$: No ignition.

Point of no return: When L intersects G in one point, if the slope of L increases we have no ignition (within that range), otherwise if the slope of L decreases, then we will always have ignition.
– This is useful for SI (petrol/gasoline) and CI (diesel) engines which want to limit and encourage autoignition respectively.
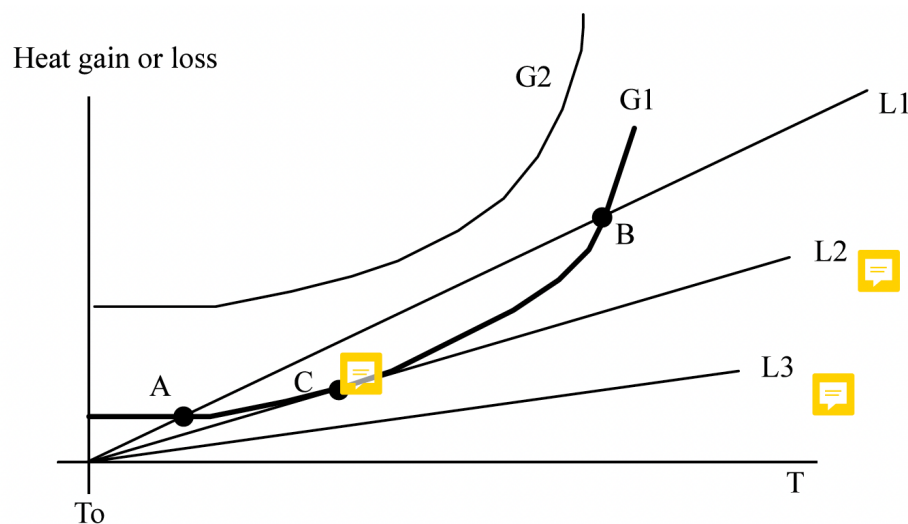
Figure 4-3. The heat generation and heat loss in a uniform mixture as a function of temperature.

– **Autoignition temperature:** The autoignition temperature is:
$$T_{ign} = T_c$$
We solve $G = L \Rightarrow \frac{\partial T}{\partial t} = 0$. This yields a 2nd order polynomial.

4.4 Worked examples

1. To calculate E_a, take logarithm of $\tau_i gn$ which yields a line (approximately and with some mental gymnastics).

2. Estimating $T_{ign} - T_0$ from Semenov's analysis:

$$T_{ign} = T_0 + \frac{R^0 T_0^2}{E}$$

5 Chapter 5: Extinction

5.1 The well stirred reactor

– Assumptions :

1. Y_k, T, P uniform inside the reactor (I guess this means isotropic?).

2. Adiabatic (no heat losses).

3. Constant pressure and volume.

4. Steady (no change with time).

5. Simple one step chemistry with $c_p = cst$.

– Equations:

• **Species balance:**
$$\dot{m}(Y_{i,in} - Y_{i,out}) = \dot{w}_i V$$

with the reaction rate

$$\dot{w}_{fuel} = -A exp(-\frac{E_a}{R^0 T_0})(\frac{M_{fuel}}{M_{fuel} M_{ox}} \rho^2 Y_f Y_{ox})$$

and

$$Y_f = Y_{f,0} - c_p \frac{T - T_0}{Q}$$

$$Y_{ox} = Y_{ox,0} - S.c_p \frac{T - T_0}{Q}$$

and the adiabatic flame temperature defined as

$$T_f = \frac{Y_f Q}{c_p} + T_0$$

• **Energy balance:**
$$\dot{m} c_p (T_{out} - T_{in}) = |Q| \dot{w}_f V$$

• **Ideal gas law:**
$$\rho = \frac{P M_{avg}}{R^0 T_0}$$

where M_{avg} is the average molar mass (taken as air: 25.58 g/mol).

By combining all equations, we obtain:

$$\underbrace{\frac{\dot{m}}{V \rho}(T - T_{in})}_{heat\ transfer,\ heat\ leaving\ reactor} = \underbrace{C f(T)}_{heat\ generation\ by\ combustion}$$

The temperature of the reactor depends only on:

1. Inlet conditions $(Y_{f,i}, Y_{ox,i}, T_i)$.

2. Pressure, volume, and mass flow rate.

3. Thermochemistry of fuel $(E/R^0, A, Q)$.

4. Mixture properties (M, c_p).

We then define the residence time as

$$t_{res} = \frac{\rho V}{\dot{m}}$$

Here, the slopes of the heat transfer terms correspond to $k_c = \frac{1}{t_{res}}$.
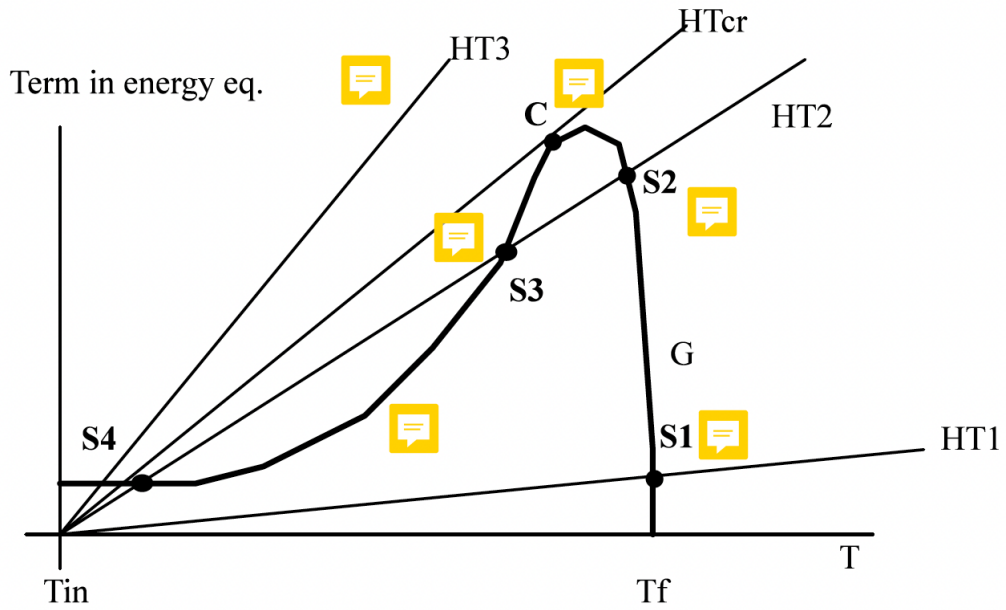
Figure 5-2. The heat generation (G) and the heat transfer term (HT) for the WSR.

– Cases:

1. $k > k_c$: The flame is quenched (extinction), because the residence time is too short and the temperature is low.

2. $k = k_c$: Blow-off limit, critical point, the combustion timescale is equal to the residence time.

3. $k < k_c$: Only S2 and S1 are realisable. For these two cases, the residence time is much longer than the combustion timescale which is desirable but can only occur at low mass flow rates (not realistic relative to practical industrial applications).

- S3: Unstable, physically unrealisable.
- S2: Low temperature = incomplete combustion.
- S1: High temperature = complete combustion.

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5.2 Worked examples

1. When T_{in} increases, the operating temperature T increases, and the reaction rate increases = resistance to extinction.
   – This is part of the reason why preheated air is used in industrial burners to help stabilisation.
   – At high altitude, P and T go down, so the residence time goes down, which may lead to blow-off at high altitudes.

2. – Q can be obtained from tables (lower calorific value).
   – Density calculated using "average" MW of air. (I made a mistake here, what I calculated was the total mass, not total <u>molar</u> mass).

$$\overline{MW} = \sum X_k M_k$$

   – S calculated with MW of oxygen, not air.
   – Y_{ox} calculated from mass fraction of oxygen, not air.
   – Energy released:
$$Q\dot{m}_f(Y_{in} - Y_{out})$$

   – Some mistakes in calculations...

6 Chapter 6: Premixed flames

6.1 Basics and equations

– Assumptions:

- $P = cst.$

- $\lambda = cst$, $c_p = cst.$

- Adiabatic system.

- Steady flow.

- One-step global chemistry.

- $Le = 1$

– Governing equations:

- **Species balance:** For fuel and oxygen.

- **Energy balance**.

- **Species mass fractions as a function of $T - T_0$**.

- **Reaction rate expression.**

- **Boundary conditions:** (Mass fractions and temperatures at inlets and outlets + $\frac{d}{dx} = 0$ at inlets and outlets).

- **Mass continuity:**
$$\rho U = \rho S_L = cst$$

- **Ideal gas law:** For density.

6.2 Flame structure

Two regions:

1. **Pre-heat zone:**

   - Largest thickness.
   - No reaction rate due to low temperatures: $\dot{w}_{fuel} = 0$
   - Only convection and diffusion terms are nonzero.
   - Heat is produced in the <u>reaction zone</u> and the **pre-heat zone** diffuses it towards the unburnt gases.
   - Between x_0 and x_I (ignition point).

2. **Reaction zone:**

- Smaller thickness.
- Higher reactivity ($\dot{w}_{fuel}$ is high and balances diffusion).
- Convection term in energy balance neglected ($\nabla(\rho_0 c_p S_L T) = 0$).

By deriving an expression for the slope at the ignition point $(\frac{dT}{dx})_{x=x_I}$ in each of these zones and then equating them, we obtain an expression for S_L.

$$S_L = \sqrt{2(\frac{\lambda}{\rho_0 c_p})(\frac{1}{\rho_0 Y_{f,0}})(\frac{RR}{T_f - T_0})}$$

where RR is the temperature-integrated reaction rate:

$$RR = \int_{T_I}^{T_f} \dot{w}_{fuel} dT$$

By plugging in the expression of RR from the reaction rate expression and simplifying:

$$S_L = \sqrt{2A\left(\frac{M_f}{M_f M_{ox}}\right)\left(\frac{\lambda}{\rho_0 c_p}\right)\left(\frac{\rho_1^2}{\rho_0}\right)\left(\frac{Y_{f,0}}{(T_f - T_0)^3}\right)\left(\frac{R^0 T_f^2}{E}\right)^3 exp\left(-\frac{E}{R^0 T_f}\right)}$$

(The ratio of densities can be replaced by a ratio of temperatures as per the ideal gas law)

This equation shows how S_L is dependent on both the diffusive (diffusivity) and chemical processes (reaction rate).

- Effects:

- *Chemistry (speed): $A \uparrow \Rightarrow S_L \uparrow$*
- *Initial temperature: $T_0^2 \uparrow \Rightarrow S_L \uparrow$*
- *Mixture strength: $\phi \uparrow \Rightarrow S_L \downarrow$*
- *Pressure: $\sqrt{P} \uparrow \Rightarrow S_L \downarrow$ (only through experiments)*

We define the flame thickness:
$$d_L = \frac{\alpha}{S_L}$$

where α is the thermal diffusivity ($\alpha = \frac{\lambda}{\rho_0 c_p}$)
and the chemical time scale as:
$$\tau_{chem} = \frac{d_L}{S_L}$$

6.3   Flammability limits

– Two limits:

- **Lean:**

  - Below 1500 K.
  - Slow chain-branching reactions.
  - Dominating chain-breaking reactions.
  - No self-sustaining combustion is possible.

- **Rich:**

  - Not enough oxygen to trigger chain-reactions.

Quenching distance – Minimum pipe diameter allowing for flame propagation is $D = 2d_L$ (otherwise quenching since the flame loses heat to the cold walls of the tube).
Spark ignition criterion – Kernel size must be roughly equal to of d_L.

6.4   Worked example

RAS.

7 Chapter 7: Non-premixed flames and droplet combustion

7.1 Non-premixed flames

7.1.1 Basics

– Characteristics:

- No flame propagation.

- Flame will exist at the interface of fuel and oxidiser streams.

- The reactants move towards the flame due to **diffusion** (and maybe advection).

– Assumptions :

1. $P = cst$.

2. Adiabatic.

3. Steady.

4. One-step global chemistry with $c_p = cst$ and $\lambda = cst$.

5. $Le = 1$.

– Equations:

- **Species:** 2D flame.

$$\rho U \frac{\partial Y_f}{\partial x} + \rho V \frac{\partial Y_f}{\partial y} = \frac{\partial}{\partial x}\left(\rho D \frac{\partial Y_f}{\partial x}\right) + \frac{\partial}{\partial y}\left(\rho D \frac{\partial Y_f}{\partial y}\right) - \dot{w}_f$$

$$\rho U \frac{\partial Y_{ox}}{\partial x} + \rho V \frac{\partial Y_{ox}}{\partial y} = \frac{\partial}{\partial x}\left(\rho D \frac{\partial Y_{ox}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\rho D \frac{\partial Y_{ox}}{\partial y}\right) - S.\dot{w}_f$$

- **Energy:** 2D energy conservation.

$$\rho U c_p \frac{\partial T}{\partial x} + \rho V c_p \frac{\partial T}{\partial y} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda \frac{\partial T}{\partial y}\right) + Q\dot{w}_f$$

- **One-step chemistry reaction rate**: $\dot{w}_f$

- **Boundary conditions:** Species mass fractions and temperatures at $x = 0, \infty$ and $y = 0, \infty$, and their spatial derivatives $\partial/\partial x$, $\partial/\partial y$.

7.2 Mixture fraction

By subtracting the fuel's species balance equation from the oxidiser's species balance equation divided by S, the source term disappears and the following scalar is **conserved**:

$$Y_f - \frac{Y_{ox}}{S}$$

We can define a second scalar called the **mixture fraction**, which corresponds to the **mass fraction of the mixture that originated in the fuel feed**:

$$\xi = \frac{\left(Y_f - \frac{Y_{ox}}{S}\right) - \left(Y_f - \frac{Y_{ox}}{S}\right)_2}{\left(Y_f - \frac{Y_{ox}}{S}\right)_1 - \left(Y_f - \frac{Y_{ox}}{S}\right)_2}$$

with: 1: fuel stream, 2: air stream.
and where the mass fractions are calculated in each respective stream.
– Naturally, $\xi_{fuel\,stream} = 1$ and $\xi_{air\,stream} = 0$.
– If no fuel or air penetrate the opposite stream:

$$\xi = \frac{Y_f - \frac{Y_{ox}}{S} + \frac{Y_{ox,2}}{S}}{Y_{f,1} + \frac{Y_{ox,2}}{S}} = \frac{Y_f - \frac{Y_{ox}}{S} + \frac{Y_{ox,0}}{S}}{Y_{f,0} + \frac{Y_{ox,0}}{S}}$$

– If no chemical reaction is happening:

$$\xi = \frac{Y_f}{Y_{f,0}}$$

7.2.1 Flame sheet model

We use the flame sheet model:

1. **Infinitely fast chemistry:** $\tau_{chem} << \tau_{diffusion}$ – no fuel can penetrate the air stream and vice versa.

2. **Reaction zone position:** The reaction zone is located where $T = T_f$ and $\phi = 1$. Therefore, the reaction zone position is characterised by a **stoichiometric mixture fraction**:
$$\xi = \xi_{st} = \frac{\frac{Y_{ox,0}}{S}}{Y_{f,0} + \frac{Y_{ox,0}}{S}}$$
since $Y_f - \frac{Y_{ox}}{S} = 0$ at stoichiometry.
If the fuel or air stream is diluted by an inert, ξ_{st} will go up or down respectively.
– According to the flame sheet model, **reaction <u>only</u> occurs at $\xi = \xi_{\mathbf{st}}$**.

7.3 State relationships and flame temperature

The temperature comes from assuming a 2-stage process as such:

1. **Inert mixing:** First, the temperature of the mixed fuel and oxygen stream (which is inert, non-reacting) is calculated:
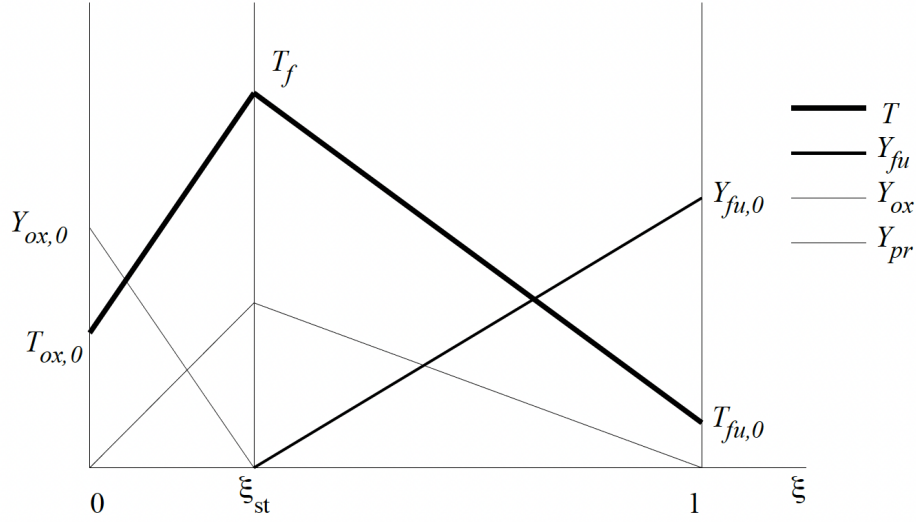$$T_{in} = \xi_{st} T_{f,0} + (1 - \xi_{st}) T_{ox,0}$$

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Figure 7-3. The mass fractions and temperature as a function of mixture fraction for a non-premixed flame.

Figure 1: The expressions for mass fractions and temperature as a function of ξ can easily be calculated by observation.

2. **Combustion:** Second, the flame temperature is calculated from the conserved scalar in the species-energy equation:

$$T_f = T_{in} + \frac{Q}{c_p}(Y_{f,st})$$

where the fuel mass fraction at stoichiometry (inert conditions) is:

$$Y_{f,st} = \xi Y_{f,0}$$

We can then estimate the flame temperature from combining both stages:

$$T_f = \underbrace{T_{ox,0} - \xi_{st}(T_{ox,0} - T_{f,0})}_{mixing} + \underbrace{\frac{Q}{c_p}\xi_{st}Y_{f,0}}_{combustion}$$

This is better explained (with better visual aid) in Benoit Fiorina's lecture notes (check appendix).

7.4 Droplet evaporation

- **Droplet mass conservation**

$$\rho_L \frac{dr_0}{dt} = -\dot{m}''_{f,0}$$

where ρ_L is the density of the liquid fuel, r_0 is the droplet diameter, and $\dot{m}''_{f,0}$ is the mass flux of the fuel at the droplet surface.

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- **Mass conservation in the gaseous phase**
  In spherical coordinates:

  – Mass balance:
  $$\rho U(4\pi r^2) = \dot{m}''_{f,0}(4\pi r_0^2)$$

  – Species balance yields the **evaporation rate** $\dot{m}''_{f,0}$:

  $$\dot{m}''_{f,0} = \frac{\rho D}{r_0} \ln\left(\frac{1 - Y_{fu,\infty}}{1 - Y_{fu,0}}\right)$$

  – **The d² law:**
  The **evaporation time** is defined as:

  $$t_{vap} = \frac{\rho_L}{8\rho D \ln(1 + B)} d_{in}^2$$

  where d_in is the initial diameter, and B is the **transfer number**:

  $$B = \frac{Y_{fu,0} - Y_{fu,\infty}}{1 - Y_{fu,0}}$$

7.5   Worked examples

1. Careful with mass fractions of non-premixed flames! They are to be calculated in each separate stream, not directly from the balanced chemical equation.
   Exhaust gas recirculation ($Y_{EGR} \approx .2$ usually) can be used to dilute the air stream, reduce the oxygen mixture fraction (and therefore flame temperatures in lean conditions) which yields shorter flames.

2. The evaporation time goes up if $Y_{f,\infty} \uparrow$ as more time is needed to vaporise the droplet cloud.
   Fine droplets are needed, otherwise evaporation time will go up with diameter size (d^2 dependency).

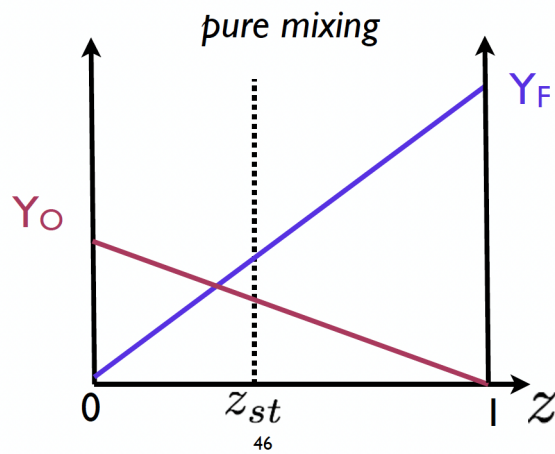# 8 Chapter 8: Pollutants

9 Appendix

S quantity:

Inert mixing (no flame)

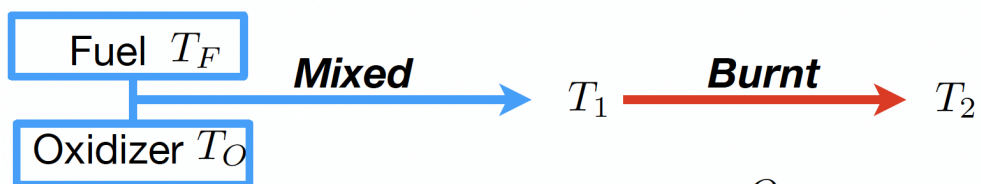$$\frac{\partial \rho Y_F}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_F) = \nabla \cdot (\rho D \nabla Y_F)$$

$$\frac{\partial \rho Y_O}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_O) = \nabla \cdot (\rho D \nabla Y_O)$$
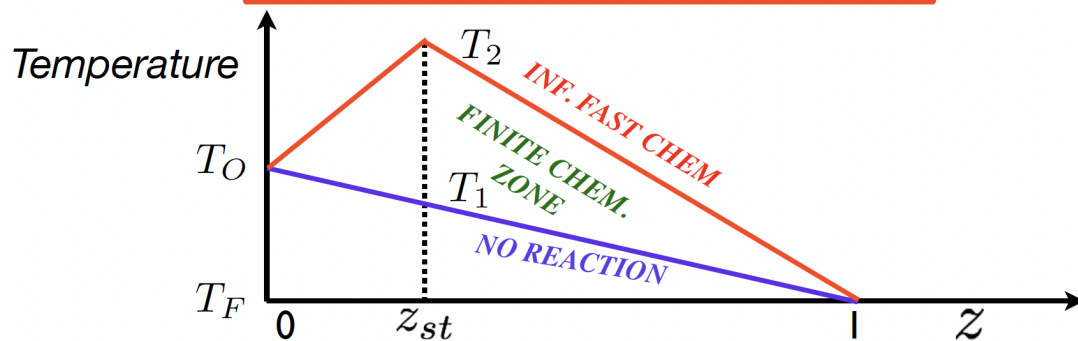
Same equation with same normalized boundary conditions

$$\frac{\partial \rho z}{\partial t} + \nabla . (\rho \mathbf{u} z) = \nabla . (\rho D \nabla z)$$

pure mixing

Y$_F$

Y$_O$

0   z_{st} 1 z

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Temperature : Mixed Is Burnt model

Fuel T_F **Mixed** $\longrightarrow$ T_1 **Burnt** $\longrightarrow$ T_2

Oxidizer T_O

$$T_1 = T_O(1-z) + T_F z \qquad T_2 = T_1 + \frac{Q_F}{C_p}Y_F^1 \ \text{ with } \ Y_F^1 = Y_F^\infty z$$

$$C_p = cst \qquad \boxed{T_2 = T_O(1-z) + T_F z + \frac{Q_F}{C_p}Y_F^\infty z}$$

$$\underbrace{\hspace{3cm}}_{MIXING} \quad \underbrace{\hspace{2.5cm}}_{COMBUSTION}$$