What is Combustion?

- What is the difference between combustion and fuel oxidation in a fuel cell?

- In contrast to isothermal chemically reacting flows
  - Heat release induces temperature increase
  - Thereby combustion is self accelerating

- Important
  - Each chemical or physical process has associated time scale

- Interaction of flow (transport) and chemistry
  - Laminar and turbulent combustion
  - New dimensionless groups (similar to Reynolds number)
    - Damköhler number, Karlovitz number, ...
Combustion Applications: Examples

- **Premixed** combustion
  - Spark-ignition engine
  - Premixed

- **Non-premixed** combustion
  - Diesel engine
  - Aircraft engine
Impact of Combustion

Demand for energy:
• Transport and electricity
• Atmospheric pollution
• Global warming
DOE’s International Energy Outlook 2011

- Increase in world wide energy consumption from 2008 until 2035: 53%
- Fossil fuels: great share (80%) of the world wide used energy
- Mineral oil remains dominating source of energy
- Traffic and transport: Share of about 25%
• Increase of renewable energy by a factor of 2
• Combustion of fossil fuels remains dominating source of energy
• Nearly 80% of energy consumption covered by fossil fuels
Greenhouse Gas Emissions

- 85% of Greenhouse gas emissions \( \text{CO}_2 \)
Sources of CO₂

Combustion of fossil fuels:
- 95% of CO₂-emissions
- 80% of all greenhouse gas-emissions
- Expected increase of CO₂ emissions: 43% from 2008 until 2035

Quelle: International Energy Outlook, 2011
Various approaches:

• Hydrogen economy
• CO₂-sequestration (Carbon Capture and Storage, CCS)
• Bio-fuels
• ...

• Increase in efficiency

Combustion Theory
New Technologies

- Challenge of concurrent optimizing of **efficiency, emissions and stability**
- Examples of new technologies
  - Aircraft turbines
    - Lean direct injection (LDI)
  - Automotive sector
    - Homogeneous charge compression ignition (HCCI, CAI)
  - Electricity generation
    - Oxy-coal combustion
    - Integrated gasification combined cycle (IGCC)
    - Flameless oxidation (FLOX) / MILD combustion
- Progress in technology increasingly supported by **numerical simulations**
- New technologies often lead to **changes in operating range**

→ **New challenges in the field of combustion theory and modeling!**
Aim of this Course

• Develop understanding of combustion processes from physical and chemical perspectives

• Fundamentals:
  – Thermodynamics
  – (Kinetics → see parallel course)
  – Fluid mechanics
  – Heat and mass transfer

• Applications:
  – Reciprocating engines
  – Gas turbines
  – Furnaces
Course Overview

Part I: Fundamentals and Laminar Flames

Part II: Turbulent Combustion

Combustion Theory

CEFRC Summer School
Princeton
June 28\textsuperscript{th} - July 2\textsuperscript{nd}, 2010

Norbert Peters\textsuperscript{1}
RWTH Aachen University
Course Overview

Part I: Fundamentals and Laminar Flames

- Introduction
- Fundamentals and mass balances of combustion systems
- Thermodynamics, flame temperature, and equilibrium
- Governing equations
- Laminar premixed flames: Kinematics and Burning Velocity
- Laminar premixed flames: Flame structure
- Laminar diffusion flames
Course Overview

Part II: Turbulent Combustion

• Turbulence
• Turbulent Premixed Combustion
• Turbulent Non-Premixed Combustion
• Modeling Turbulent Combustion
• Applications
Fundamentals and Mass Balances of Combustion Systems

Combustion Summer School

2014

Prof. Dr.-Ing. Heinz Pitsch
The final state (after very long time) of a homogeneous system is governed by the classical laws of thermodynamics!

Prerequisites:

- Definitions of concentrations and thermodynamic variables
- Mass and energy balances for multicomponent systems
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  - Stoichiometry
  - Mixture Fraction
Definitions, Equation of State, Mass Balance

- In chemical reactions mass and chemical elements are conserved
- Combustion always in (gas) mixtures

The mole fraction

- Multi-component system with $k$ different chemical species
- Mole: $6.0236 \cdot 10^{23}$ molecules are defined as one mole $\rightarrow$ Avogadro number $N_A$
- Number of moles of species $i$: $n_i$
- Total number of moles:
  \[
  n_S = \sum_{i=1}^{k} n_i
  \]
- Mole fraction of species $i$:
  \[
  X_i = \frac{n_i}{n_S}, \quad i = 1, 2, \ldots, k
  \]
The mass fraction

- Mass $m_i$ of all molecules of species $i$ is related to its number of moles by
  \[ m_i = W_i n_i, \quad i = 1, 2, \ldots, k \]
  where $W_i$ is the molecular weight of species $i$

- Total mass of all molecules in the mixture:
  \[ m = \sum_{i=1}^{k} m_i \]

- Mass fraction of species $i$:
  \[ Y_i = \frac{m_i}{m}, \quad i = 1, 2, \ldots, k \]

- Mean molecular weight $W$:
  \[ W = \sum_{i=1}^{k} W_i X_i = \left[ \sum_{i=1}^{k} \frac{Y_i}{W_i} \right]^{-1} \]

- Mass fraction and mole fraction:
  \[ Y_i = \frac{W_i}{W} X_i \]
The mass fraction of elements

- Mass fractions of elements are very useful in combustion

  - Mass of the species changes due to chemical reactions, but mass of the elements is conserved

- Number of atoms of element $j$ in a molecule of species $i$: $a_{ij}$

- Mass of all atoms $j$ in the system:

  $$ m_j = \sum_{i=1}^{k} a_{ij} \frac{W_j}{W_i} m_i, \quad j = 1, 2, \ldots, k_e $$

  where $k_e$ is the total number of elements in the system, $W_j$ is molecular weight of element $j$
The mass fraction of elements

- The mass fraction of element $j$ is then

$$Z_j = \frac{m_j}{m} = \sum_{i=1}^{k} \frac{a_{ij} W_j}{W_i} Y_i = \frac{W_j}{W} \sum_{i=1}^{k} a_{ij} X_i, \quad j = 1, 2, \ldots, k_e,$$

- From the definitions above it follows

$$\sum_{i=1}^{k} X_i = 1, \quad \sum_{i=1}^{k} Y_i = 1, \quad \sum_{j=1}^{k_e} Z_j = 1$$
The partial molar density (concentration)

- Number of moles per volume $V$ or partial molar density, the concentration:

$$[X_i] = \frac{n_i}{V}, \quad i = 1, 2, \ldots, k$$

- Total molar density of the system is then

$$\frac{n_s}{V} = \sum_{i=1}^{k} [X_i]$$
The Partial Density

• The density and the partial density are defined

\[ \rho = \frac{m}{V}, \quad \rho_i = \frac{m_i}{V} = \rho Y_i, \quad i = 1, 2, \ldots, k \]

• The partial molar density is related to the partial density and the mass fraction by

\[ [X_i] = \frac{\rho_i}{W_i} = \frac{\rho Y_i}{W_i}, \quad i = 1, 2, \ldots, k \]

(relation often important for evaluation of reaction rates)
The thermal equation of state

- In most combustion systems, thermally ideal gas law is valid

- Even for high pressure combustion this is a sufficiently accurate approximation, because the temperatures are typically also very high

- In a mixture of ideal gases the molecules of species $i$ exert on the surrounding walls of the vessel the partial pressure

$$p_i = \frac{n_i \mathcal{R} T}{V} = [X_i] \mathcal{R} T = \rho \frac{Y_i}{W_i} \mathcal{R} T, \quad i = 1, 2, \ldots, k$$

- Universal gas constant equal to

$$\mathcal{R} = 8.3143 \text{ J/mol/K} = 82.05 \text{ atm cm}^3/\text{mol/K}$$
Dalton's law

- For an ideal gas the total pressure is equal to the sum of the partial pressures.

- Thermal equation of state for a mixture of ideal gases

\[ p = \sum_{i=1}^{k} p_i = n_s \frac{RT}{V} = \rho RT \]

- From this follows

\[ p_i = pX_i, \quad i = 1, 2, \ldots, k \]

- And for the volume

\[ V = n_i \frac{RT}{p_i} = n \frac{RT}{p} \]
Example: Methane/Air Mixture

- Known: CH$_4$-air-mixture; 5 mass percent CH$_4$, 95 mass percent air
  Air: 21% (volume fraction) O$_2$, 79% N$_2$ (approximately)
- Unknown: Mole fractions and element mass fractions
- Solution:
  - Molar masses: $M_{O_2} \approx 32$ g/mol, $M_{N_2} \approx 28$ g/mol, $M_{CH_4} \approx 16$ g/mol
  
  - Mass fractions in the air: $Y_i = \frac{M_i}{M} X_i$
  
  $Y_{O_2,L} = \frac{M_{O_2} X_{O_2,L}}{M_{O_2} X_{O_2,L} + M_{N_2} X_{N_2,L}} \approx 0.232$, $Y_{N_2,L} = 1 - Y_{O_2,L} \approx 0.768$

  - In the mixture: $Y_{O_2} = 0.95 Y_{O_2,L} = 0.22$, $Y_{N_2} = 0.95 Y_{N_2,L} = 0.73$

  - Mean molar mass: $M = \left[ \sum_{i=1}^{3} \frac{Y_i}{M_i} \right]^{-1} = 27.5$ g/mol
Example: Methane/Air Mixture

• Mole fractions of Components: \( X_i = \frac{M}{M_i} Y_i \)

\[
X_{\text{CH}_4} = 0.09, \quad X_{\text{O}_2} = 0.19, \quad X_{\text{N}_2} = 0.72
\]

• Molar mass of elements: \( M_H \approx 1 \text{ g/mol}, \quad M_C \approx 12 \text{ g/mol} \)

• with:

\[
Z_j = \sum_{i=1}^{3} \frac{a_{ij}}{M_i} M_j Y_i
\]

• Mass fractions of elements: \( Z_H = 0.0125, \quad Z_C = 0.0375, \quad Z_O = Y_{\text{O}_2}, \quad Z_N = Y_{\text{N}_2} \)

• Simplification: Whole numbers for values of the molar masses
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Elementary and Global Reactions

- Distinction between **elementary reactions** and **global reactions** important!

- **Elementary reactions**
  - Describes actual micro-process of chemical reaction
  - Only take place, if collisions between reactants take place
  - Reaction velocities can be determined experimentally oder theoretically

- **Global reactions**
  - Conversion of educts to products
  - Ratios of amounts of substance
  - Does not represent a chemical micro-process
  - Temporal process of the reaction cannot be given

\[
H^\circ + O_2 \rightarrow OH^\circ + O^\circ \]

\[
2H_2 + O_2 = 2H_2O
\]
Elementary Reactions

- Observe the conservation of elements
- Chemical changes due to collisions of components
- Transition from educts to products symbolized by arrow
- Example: Bimolecular elementary reaction

\[ \text{H}^\circ + \text{O}_2 \rightarrow \text{OH}^\circ + \text{O}^\circ \]

- Elementary reactions also proceed backwards:

\[ \text{H}^\circ + \text{O}_2 \rightleftarrows \text{OH}^\circ + \text{O}^\circ \]

- Often symbolized by a double arrow:
Global reactions

• Conservation of elements

• Global ratios of amounts of substance

• Do not take place on atomic scale

• Global balance of a variety of elementary reactions

• Equality sign for global reactions

• Example for global reaction: \[ 2H_2 + O_2 = 2H_2O \]

meaning that 2 mol H₂ react with 1 mol O₂, yielding 2 mol H₂O
Global reactions

- **Multiples** of the equation are also valid:

  \[ \text{H}_2 + \frac{1}{2}\text{O}_2 = \text{H}_2\text{O} \]

  – This does not hold for elementary reactions!

- Multiplication of the equation of the global reaction by the molar masses
  \[ \rightarrow \quad \text{Mass balance during combustion} \]

- Example: Combustion of \( \text{H}_2 \) using the foregoing equation

  \[ 2\;\text{g}\;\text{H}_2 + 16\;\text{g}\;\text{O}_2 = 18\;\text{g}\;\text{H}_2\text{O} \]
Global reactions

• Stoichiometric coefficient of reactants $i$: $\nu_i$

• Stoichiometric coefficient of products $i$: $\nu_i^{\prime\prime}$

• Stoichiometric coefficient of a component (only for global reactions): $\nu_i := \nu_i^{\prime\prime} - \nu_i^{\prime}$

• Note:
  – Stoichiometric coefficients $\nu_i$ of the educts are negative!
  – Whereas $\nu_i^{\prime}$ are defined to be positive!
Global reactions

Formulation of global reactions:

- Combustion of hydrocarbon fuel or an alcohol

\[ \nu'_B B + \nu'_O O_2 = \nu''_C CO_2 + \nu''_H H_2O \]

- Atoms in the fuel: Carbon, hydrogen and oxygen
  - Number of atoms in the fuel \( a_{BC}, a_{BH}, a_{BO} \)

- Stochiometric coefficients of the global reaction are derived from \( \nu'_B \)
  - Balances of atoms

  - C:
    \[ \nu''_C = a_{BC} \nu'_B \]
  - H:
    \[ \nu''_H = a_{BH} \nu'_B / 2 \]
  - O:
    \[ \nu'_O = \nu''_C + \nu''_H / 2 - a_{BO} \nu'_B / 2 \]

- Example: \( CH_4 + 2O_2 = CO_2 + 2H_2O \)

\[ a_{BC} = 1, \quad a_{BH} = 4, \quad a_{BO} = 0, \quad \nu_B = 1 \]
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Coupling functions

Global reaction, e.g.: \( \nu_1 \text{F} + \nu_2 \text{O} = \nu_3 \text{P} \)

- Conversion of:
  - \( n_1 \) moles of component 1
  - \( n_i \) moles of component \( i \)

- Reaction has taken place \( n_1/\nu_1 \) or \( n_i/\nu_i \) times \( \rightarrow n_1/\nu_1 = n_i/\nu_i \)

- Differential notation:
  \[
  \frac{dn_i}{\nu_i} = \frac{dn_1}{\nu_1}, \quad \frac{dm_i}{\nu_i M_i} = \frac{dm_1}{\nu_1 M_1}, \quad \frac{dY_i}{\nu_i M_i} = \frac{dY_1}{\nu_1 M_1} \quad (i = 1, 2, ..., n)
  \]

- Integrating, e.g. for fuel and oxygen from the unburnt state
  \( \rightarrow \) Coupling function:

\[
\frac{Y_{O_2} - Y_{O_2,u}}{\nu'_{O_2} M_{O_2}} = \frac{Y_B - Y_{B,u}}{\nu'_B M_B}
\]
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Stoichiometry

• Stoichiometric:
  - Fuel-to-oxygen ratio such that both are entirely consumed when combustion to CO$_2$ and H$_2$O is completed

• For example,
  - Global reaction describing combustion of a single component hydrocarbon fuel C$_m$H$_n$ (subscript F for fuel)

$$\nu'_F C_m H_n + \nu'_O O_2 = \nu''_C CO_2 + \nu''_H H_2O$$

- Stoichiometric coefficients are

$$\nu'_F = 1, \quad \nu'_O = m + \frac{n}{4}, \quad \nu''_C = m \quad \nu''_H = \frac{n}{2}$$

where $\nu'_F = 1$ may be chosen arbitrarily to unity
Stoichiometric Mass Ratio

- Mole number ratio for stoichiometric condition

\[ \frac{n_{O_2,u}}{n_{F,u}} \mid_{st} = \frac{\nu'_O}{\nu'_{F}} \]

or in terms of mass fractions

\[ \frac{Y_{O_2,u}}{Y_{F,u}} \mid_{st} = \frac{\nu'_O W_{O_2}}{\nu'_{F} W_{F}} = \nu \]

where \( \nu \) is called the stoichiometric mass ratio

- Typical value: Methane: \( \nu = 4 \)
- Mass ratio \( \nu \)
  - Fuel and oxidizer are both consumed when combustion is completed
Stoichiometric Mass Ratio

• This is consistent with coupling function, since

\[
\frac{Y_{O_2} - Y_{O_2,u}}{\nu'_{O_2} W_{O_2}} = \frac{Y_F - Y_{F,u}}{\nu'_{F} W_{F}}
\]

leads to

\[
\nu Y_F - Y_{O_2} = \nu Y_{F,u} - Y_{O_2,u}
\]

• Complete consumption of fuel and oxygen

\[
Y_F = Y_{O_2} = 0
\]

leads to

\[
\left. \frac{Y_{O_2,u}}{Y_{F,u}} \right|_{st} = \frac{\nu'_{O_2} W_{O_2}}{\nu'_{F} W_{F}} = \nu
\]
*Extra: Minimum oxygen requirement

- Minimum oxygen requirement (molar): $o_{\text{min},m}$

  $\rightarrow$ Fuel/air mole number ratio before combustion at stoichiometric conditions

  $\rightarrow$ Ratio of the stoichiometric coefficients

  $$o_{\text{min},m} = \frac{n_{O_2,u}}{n_{B,u}}|_{st} = \frac{X_{O_2,u}}{X_{B,u}}|_{st} = \frac{\nu'_{O_2}}{\nu'_{B}}$$

- Minimum oxygen requirement (mass): $o_{\text{min}}$

  $$o_{\text{min}} = \frac{m_{O_2,u}}{m_{B,u}}|_{st} = \frac{X_{O_2,u}}{X_{B,u}}|_{st} \cdot \frac{M_{O_2}}{M_{B}} = \frac{\nu'_{O_2} M_{O_2}}{\nu'_{B} M_{B}} \equiv \nu$$
*Extra: Minimum air requirement

- Minimum air requirement:
  - Mass of air per mass of fuel in complete combustion

\[ \ell_{\text{min}} \]

- Relation between minimum oxygen and minimum air requirement:

\[ \ell_{\text{min}} = \frac{o_{\text{min}}}{Y_{O_2,\text{Luft}}} \quad , \quad \ell_{\text{min},m} = \frac{o_{\text{min},m}}{X_{O_2,\text{Luft}}} \Rightarrow \ell_{\text{min}} = \frac{o_{\text{min}}}{0,232} \quad , \quad \ell_{\text{min},m} = \frac{o_{\text{min},m}}{0,21} \]

with:
- Mass fraction \( Y_{O_2,\text{air}} = 0,232 \)
- Mole fraction \( X_{O_2,\text{air}} = 0,21 \)
The equivalence ratio

- The **equivalence ratio** is the ratio of fuel to oxidizer ratio in the unburnt to that of a stoichiometric mixture.

- For combustion with oxygen,

\[ \phi = \frac{Y_{F,u}/Y_{O_2,u}}{(Y_{F,u}/Y_{O_2,u})_{st}} = \frac{\nu Y_{F,u}}{Y_{O_2,u}} \]

- Can be written also in terms of
  - Fuel to air ratio
  - Mole fractions

- Stoichiometric mass ratio \( \nu \) obtained from global reaction
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The mixture fraction

• Equivalence ratio important parameter in combustion
• Mixture fraction quantifies local fuel-air ratio in non-premixed combustion

• Consider two separate feed streams of
  – Fuel
  – Oxidizer (air, pure oxygen)
• Streams mix and burn

• Fuel stream
  – Often consists of one component only
  – In general does not contain oxidizer
• Oxidizer stream
  – Generally does not contain fuel
The mixture fraction

In the following:
• Fuel stream: Subscript 1
• Oxidizer stream: Subscript 2

Definition mixture fraction
• Mass fraction of the fuel stream in the mixture:

\[ Z = \frac{m_1}{m_1 + m_2} \]

where \( m_1 \) and \( m_2 \) are the local mass originating from the individual streams

• Mixture fraction always between zero and one
• Fuel stream: \( Z = 1 \)
• Oxidizer stream: \( Z = 0 \)
The mixture fraction

• Mass fraction of fuel in the fuel stream: $Y_{B,1}$
• Mass fraction of oxygen in the oxidizer stream: $Y_{O2,2}$

➢ Before combustion:
  Dividing $m_{B,u} = Y_{B,1} m_1$ by the total mass flow, yields

→ Mixture fraction linear with fuel mass

\[
Y_{B,u} = Y_{B,1} Z
\]
\[
Y_{O2,u} = Y_{O2,2} (1 - Z)
\]

➢ Coupling function:

\[\nu Y_B - Y_{O2} = \nu Y_{B,u} - Y_{O2,u}\]

\[
Z = \frac{\nu Y_B - Y_{O2} + Y_{O2,2}}{\nu Y_{B,1} + Y_{O2,2}}
\]

Note: Index B means fuel
The mixture fraction

- Mixture fraction:
  \[ Z = \frac{\nu Y_B - Y_{O_2} + Y_{O_2,2}}{\nu Y_{B,1} + Y_{O_2,2}} \]

- For *stoichiometric* composition:
  \[ \Rightarrow \quad \text{The first two terms in the numerator have to cancel out} \]

  ➢ Stoichiometric mixture fraction:

  \[ Z_{st} = \frac{Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}} \]

  \[ Z_{st} = [1 + \nu \frac{Y_{B,1}}{Y_{O_2,2}}]^{-1} = [1 + \frac{\nu'_{O_2} M_{O_2} Y_{B,1}}{\nu'_{B} M_{B} Y_{O_2,2}}]^{-1} \]
Mixture fraction definition by Bilger

- Consider elements C, H, O in combustion of a $C_mH_n$ fuel with oxygen or air

$$\nu_F C_mH_n + \nu_{O2} O_2 = \text{Products}$$

- Changes in elements

$$\frac{dn_C}{m \nu_F} = \frac{dn_H}{n \nu_F} = \frac{dn_O}{2 \nu_{O2}}$$

or in terms of element mass fraction

$$\frac{dZ_C}{\nu_F m W_C} = \frac{dZ_H}{\nu_F n W_H} = \frac{dZ_O}{\nu_{O2} W_{O2}}$$

- Coupling function:

$$\beta = \frac{Z_C}{\nu'_F m W_C} + \frac{Z_H}{\nu'_F n W_H} - 2 \frac{Z_O}{\nu'_{O2} W_{O2}}$$

→ Changes in $\beta$ should vanish
Mixture fraction definition by Bilger

• Normalizing this such that $Z = 1$ in the fuel stream and $Z = 0$ in the oxidizer stream, one obtains Bilger's definition

$$Z = \frac{\beta - \beta_2}{\beta_1 - \beta_2}$$

or

$$Z = \frac{Z_C/(mW_C) + Z_H/(nW_H) + 2(\gamma_{O_2,B} - \gamma_O)/(\gamma'_{O_2} W_{O_2})}{Z_{C,1}/(nW_C) + Z_{H,1}/(mW_H) + 2\gamma_{O_2,B}/(\gamma'_{O_2} W_{O_2})}$$

• Because elements are conserved during combustion, element mass fractions calculated from

$$Z_j = \frac{m_j}{m} = \sum_{i=1}^{k} \frac{a_{ij} W_j}{W_i} Y_i = \frac{W_j}{W} \sum_{i=1}^{k} a_{ij} X_i, \quad j = 1, 2, \ldots, k_e,$$

do not change
Relation of mixture fraction with equivalence ratio

- **Fuel-air equivalence ratio**

\[ \phi = \frac{Y_{F,u}/Y_{O_2,u}}{(Y_{F,u}/Y_{O_2,u})_{st}} = \frac{\nu Y_{F,u}}{Y_{O_2,u}} \]

- Introducing \( Y_{F,u} = Y_{F,1}Z \) and \( Y_{O_2,u} = Y_{O_2,2}(1 - Z) \)

into \( \nu Y_F - Y_{O_2} = \nu Y_{F,u} - Y_{O_2,u} \)

leads with \( \frac{\nu Y_{F,1}}{Y_{O_2,2}} = \frac{1 - Z_{st}}{Z_{st}} \)

to a unique relation between the equivalence ratio and the mixture fraction

\[ \phi = \frac{Z \ (1 - Z_{st})}{1 - Z \ Z_{st}} \]
The equivalence ratio

• This relation is also valid for multicomponent fuels (see exercise below)

• It illustrates that the mixture fraction is simply another expression for the local equivalence ratio

Exercise:

- The element mass fractions $Z_{H,F}, Z_{C,F}$ of a mixture of hydrocarbons and its mean molecular weight $W$ are assumed to be known

- Determine its stoichiometric mixture fraction in air

- Hint: $Z_{H,F} = nW_H/W, \quad Z_{C,F} = mW_C/W$
Profiles of $Y_F$ and $Y_{O_2}$ in the unburnt gas

$$Y_{B,u} = Y_{B,1} Z$$

$$Y_{O_2,u} = Y_{O_2,2} (1 - Z)$$
Diffusion Flame Structure at Complete Conversion

- **Stoichiometric composition**

  \[ Z_{st} = \frac{Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}} \]

- **If** \( Z < Z_{st} \), **fuel is deficient**
  - Mixture is **fuel lean**
  - Combustion terminates when all fuel is consumed: \( Y_{F,b} = 0 \)
    (burnt gas, subscript \( b \))

- **Remaining oxygen mass fraction in the burnt gas** is calculated from

  \[ Z = \frac{\nu Y_{F} - Y_{O_2} + Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}} \]

  as

  \[ Y_{O_2,b} = Y_{O_2,2} \left(1 - \frac{Z}{Z_{st}}\right), \quad Z \leq Z_{st} \]
• If $Z > Z_{st}$ oxygen is deficient
  • Mixture is fuel rich

• Combustion then terminates when all the oxygen is consumed: $Y_{O_2,b} = 0$

leading to

$$Y_{F,b} = Y_{F,1} \frac{Z - Z_{st}}{1 - Z_{st}}, \quad Z \geq Z_{st}$$
For hydrocarbon fuel $C_mH_n$, the element mass fractions in the unburnt mixture are

$$Z_C = m \frac{W_C}{W_F} Y_{F,u}, \quad Z_H = n \frac{W_H}{W_F} Y_{F,u}, \quad Z_O = Y_{O_2,u}$$

For the burnt gas they are for the hydrocarbon fuel considered above

$$Z_C = m \frac{W_C}{W_F} Y_{F,b} + \frac{W_C}{W_{CO_2}} Y_{CO_2,b}$$

$$Z_H = n \frac{W_H}{W_F} Y_{F,b} + 2 \frac{W_H}{W_{H_2O}} Y_{H_2O,b}$$

$$Z_O = 2 \frac{W_O}{W_{O_2}} Y_{O_2,b} + 2 \frac{W_O}{W_{CO_2}} Y_{CO_2,b} + \frac{W_O}{W_{H_2O}} Y_{H_2O,b}$$

Elements are conserved, hence $Z_{j,u} = Z_{j,b}$
This leads with \( Y_{F,u} = Y_{F,1}Z \) and \( Y_{F,b} = 0 \) for \( Z \leq Z_{st} \)

and

\[
Z = \frac{\nu Y_F - Y_{O_2} + Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}} \quad \text{for} \quad Z \geq Z_{st}
\]

to piecewise linear relations of the product mass fractions in terms of \( Z \):

\[
Z \leq Z_{st} : \quad Y_{CO_2,b} = Y_{CO_2, st} \frac{Z}{Z_{st}}, \quad Y_{H_2O,b} = Y_{H_2O, st} \frac{Z}{Z_{st}}
\]

\[
Z \geq Z_{st} : \quad Y_{CO_2,b} = Y_{CO_2, st} \frac{1 - Z}{1 - Z_{st}}, \quad Y_{H_2O,b} = Y_{H_2O, st} \frac{1 - Z}{1 - Z_{st}}
\]

where

\[
Y_{CO_2, st} = Y_{F,1} Z_{st} \frac{m W_{CO_2}}{W_F}
\]
Profiles in the burning mixture

Burke-Schumann Solution:

Infinitely fast, irreversible chemistry
Summary

Part I: Fundamentals and Laminar Flames

• Introduction
• Fundamentals and mass balances of combustion systems
• Thermodynamics, flame temperature, and equilibrium
• Governing equations
• Laminar premixed flames: Kinematics and Burning Velocity
• Laminar premixed flames: Flame structure
• Laminar diffusion flames

• Definitions, Equation of State, Mass Balance
• Elementary and Global Reactions
• Coupling Functions
• Stoichiometry
• Mixture Fraction