Combustion Theory and Applications in CFD
Princeton Combustion Summer School
2018

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Combustion Applications

Mobility & Transport
Combustion Applications

Power Generation

Mobility & Transport

Institute for Combustion Technology | Heinz Pitsch
Combustion Applications

Power Generation

Mobility & Transport

Industry & Household
Combustion Applications

Power Generation

Fire Safety & Explosions

Mobility & Transport

Industry & Household

NIST: Safe Refrigerants
Combustion Applications

Combustion is omnipresent!

But causes emissions of

- Harmful pollutants
- Greenhouse gases

Design challenge

- Combustion extremely complex, multi-scale & multi-physics
- Devices usually big and high power
- Measurement in severe environments difficult

➡ Computational engineering very important
Combustion Science

• Combustion research started many years ago

• Why is combustion science still important?
• Why is combustion science interesting?
• HPC as an important step
World Energy Consumption

- Increase in world wide energy consumption from 2012 until 2040: 50%
- Fossil fuels > 75% by 2040

Large numbers

- 120 million tons daily CO₂ emissions in 2040 ➞ 13 kg daily per person
- 10 billion liter daily fuel consumption ➞ 1.3 liter daily liquid fuel use

Clean combustion extremely important!
IEA’s World Energy Outlook 2015

Primary Energy Demand by Region & Source in 2040

China: 2.9 toe per person
United States: 6.7 toe per person
India: 1.5 toe per person
European Union: 2.8 toe per person
Africa: 1.1 toe per person

Note: *Computed as energy_{2040} / people_{2017}
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Middle East: 0.8 toe per person
Southeast Asia: 0.7 toe per person
Latin America: 0.6 toe per person
Russia: 0.5 toe per person

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- Russia

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DOE’s International Energy Outlook 2016

Transport Sector World Energy Consumption by Source

- Fraction of Battery Electric Vehicle (BEV) in 2040 still small

→ 6% BEV for 450 scenario
DOE’s International Energy Outlook 2016

World Net Electricity Generation by Source

- For positive effect of BEV, electric power should be from renewable sources
GIH emissions can be reduced by considering
1. Energy use
2. Primary energy
3. Conversion process
Mitigation of GHG Emissions

Energy Use

Opportunities

- Electrification, but
  - electrical power has to be from renewable sources
- Also, not all relevant applications can be electrified, i.e.
  - industrial processes requiring high process temperatures
  - applications requiring high energy densities
  - …
Mitigation of GHG Emissions

Primary Energy and Conversion Process

Opportunities

• Cleaner fuels, e.g. natural gas
  ➡ Almost 50% lower specific carbon emissions compared with coal

• Biofuels
  ➡ CoE Tailor-Made Fuels from Biomass

• Carbon-free fossil fuel combustion
  ➡ CCS, CCU (SFB Oxyflame)

• Renewable electricity
  ➡ Storage
     • E-fuels
     • Ammonia
     • Hydrogen
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
Various approaches:

- Hydrogen economy
- CO$_2$-sequestration (Carbon Capture and Storage, CCS)
- Bio-fuels
- ...
- Increase in efficiency
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
- FlameMaster flame calculator

Request access and download at https://www.itv.rwth-aachen.de/index.php?id=flamemaster
Course Overview

Part II: Turbulent Combustion

• Turbulence
• Turbulent Premixed Combustion
• Turbulent Non-Premixed Combustion
• Turbulent Combustion Modeling
• Applications
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
- Burke-Schumann Solution
• 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:

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

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

- Mass fraction of element $j$ is then

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

- From 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

• Density and partial density are defined

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

• Partial molar density is related to partial density and 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 ideal gas 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 mixture of ideal gases, molecules of species $i$ exert on the surrounding walls of the vessel the partial pressure

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

- 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

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

- 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: CH₄-air-mixture; 5 mass percent CH₄, 95 mass percent air
  Air: 21% (volume fraction) O₂, 79% N₂ (approximately)
- Unknown: Mole fractions and element mass fractions
- Solution:
  - Molar masses: $M_{O_2} \approx 32 \text{ g/mol}$, $M_{N_2} \approx 28 \text{ g/mol}$, $M_{CH_4} \approx 16 \text{ g/mol}$
  - Mass fractions in the air: $Y_i = \frac{M_i}{M} X_i$
    
    $$Y_{O_2,L} = \frac{M_{O_2} X_{O_2,L}}{M_{O_2} X_{O_2,L} + M_{N_2} X_{N_2,L}} \approx 0.232, \quad Y_{N_2,L} = 1 - Y_{O_2,L} \approx 0.768$$
  - In the mixture: $Y_{O_2} = 0.95 \quad Y_{O_2,L} = 0.22, \quad Y_{N_2} = 0.95 \quad Y_{N_2,L} = 0.73$
  - Mean molar mass: $M = \left[ \sum_{i=1}^{3} \frac{Y_i}{M_i} \right]^{-1} = 27.5 \text{ g/mol}$
*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:

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

- 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
  – Describe actual micro-process of chemical reaction
  – Only take place, if collisions between reactants take place
  – Reaction velocities can be determined experimentally oder theoretically

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

• 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

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

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

• Often symbolized by a double arrow:

\[ \text{H}^\circ + \text{O}_2 \rightleftharpoons \text{OH}^\circ + \text{O}^\circ \]
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: \[ 2\text{H}_2 + \text{O}_2 = 2\text{H}_2\text{O} \]

  meaning that 2 mol \( \text{H}_2 \) react with 1 mol \( \text{O}_2 \), yielding 2 mol \( \text{H}_2\text{O} \)
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

  \[ \rightarrow \text{ Mass balance during combustion } \]

• Example: Combustion of H\textsubscript{2} using the foregoing equation

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

- Stoichiometric coefficient of reactants $i$: $\nu'_i$
- Stoichiometric coefficient of products $i$: $\nu''_i$
- Example:
  $\text{CH}_4 + 2\text{O}_2 = \text{CO}_2 + 2\text{H}_2\text{O}$
  $- \nu'_{\text{CH}_4} = 1, \quad \nu''_{\text{H}_2\text{O}} = 2$

- Stoichiometric coefficient of a component (only for global reactions):
  $\nu_i := \nu''_i - \nu'_i$
- Example:
  $\frac{dC_i}{dt} = \nu_i \omega$
  - Rate of change for reactants negative

- Note:
  - Stoichiometric coefficients $\nu_i$ of reactants are negative!
  - $\nu'_i$ 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: \( \nu''_{CO_2} = a_{BC} \nu'_B \)
  - H: \( \nu''_{H_2O} = a_{BH} \nu'_B / 2 \)
  - O: \( \nu''_{O_2} = \nu''_{CO_2} + \nu''_{H_2O} / 2 - a_{BO} \nu'_B / 2 \)

- 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

Example: Global reaction \[ 4 \text{H}_2 + 2\text{O}_2 = 4\text{H}_2\text{O} \]

• Consider conversion of 8 moles of H\(_2\)
  • How many moles of O\(_2\) have been converted?
  • Reaction has taken place how many times?

• In equations:

\[
\frac{dC_i}{dt} = \nu_i \omega \quad \text{with} \quad C_i = \frac{n_i}{V}
\]

or

\[
\frac{dn_i}{\nu_i} \frac{dt}{dt} = \omega V
\]

→ Change of \(n_i/\nu_i\) same for all species
Global reaction, e.g.: \( \nu_1 F + \nu_2 O = \nu_3 P \)

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

- Integrating, e.g. for fuel and oxygen from the unburnt state
  \( \Rightarrow \) Coupling function:
  \[
  \frac{Y_{O_2} - Y_{O_2,u}}{\nu'_O M_{O_2}} = \frac{Y_{B} - Y_{B,u}}{\nu'_B M_{B}}
  \]
Coupling functions – Example H₂

**Coupling function:**

\[
\frac{Y_{O_2} - Y_{O_2,u}}{\nu'_{O_2} M_{O_2}} = \frac{Y_B - Y_{B,u}}{\nu'_{B} M_{B}} \quad \Leftrightarrow \quad \Delta Y_{O_2} = \nu \Delta Y_B
\]

**Example:**

A closed system contains H₂ und O₂. Through combustion reactions, 1 kg H₂ is consumed. What mass of O₂ has been converted? How much air is needed?

1. Multiply coupling function by total mass

\[
\Delta Y_{O_2} = \nu \Delta Y_B \quad \Rightarrow \quad \Delta m_{O_2} = \nu \Delta m_B
\]

2. Determination of \( \nu \)

\[
\begin{align*}
\text{H}_2 + \frac{1}{2} \text{O}_2 & = \text{H}_2\text{O} \\
\nu & = \frac{0.5 \cdot 32 \text{g/mol}}{2 \text{g/mol}} = 8
\end{align*}
\]

\( \Rightarrow \) For burning 1kg H₂, 8kg \( \times \frac{76.7}{23.3} = 26.3 \) kg of air is needed
Example: How much CO$_2$ is formed when burning 1 liter of gasoline?

Assumptions: Density of liquid gasoline is roughly 0.75 kg/l
Gasoline can be approximated by iso-octane

1. Starting point: One-step global reaction $\text{C}_8\text{H}_{18} + 12.5 \text{ O}_2 = 8 \text{ CO}_2 + 9 \text{ H}_2\text{O}$
2. Coupling function between fuel and CO$_2$

$$\frac{dm_B}{\nu'_B M_B} = \frac{dm_{CO_2}}{\nu''_{CO_2} M_{CO_2}}$$

3. Integrations leads to

$$\Delta m_{CO_2} = \frac{\nu''_{CO_2} M_{CO_2}}{\nu'_B M_B} \Delta m_B$$

→ During combustion of 1 liter Gasoline, 2.3 kg CO$_2$ are produced
→ Under standard conditions, this is roughly 1.3 m$^3$ CO$_2$
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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)

\[
\nu'_F C_m H_n + \nu'_O_2 O_2 = \nu''_C O_2 CO_2 + \nu''_H_2 O H_2 O
\]

- Stoichiometric coefficients are

\[
\nu'_F = 1, \quad \nu'_O_2 = m + \frac{n}{4}, \quad \nu''_C O_2 = m \quad \nu''_H_2 O = \frac{n}{2}
\]

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

- Mole number ratio for stoichiometric condition

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

or in terms of mass fractions

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

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

- Typical values: Methane: \( \nu = 4 \); N-Dodecane: \( \nu = 3.5 \)
- 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

\[
\frac{Y_{O_2,u}}{Y_{F,u}} \bigg|_{st} = \frac{\nu'_{O_2} W_{O_2}}{\nu'_{F} W_F} = \nu
\]
• Minimum oxygen requirement (molar): \( o_{\text{min},m} \)

\[ \rightarrow \text{Fuel/air mole number ratio before combustion at stoichiometric conditions} \]

\[ \rightarrow \text{Ratio of the stoichiometric coefficients} \]

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

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

\[ o_{\text{min}} = \frac{m_{O_2,u}}{m_{B,u}} \bigg|_{st} = \frac{X_{O_2,u}}{X_{B,u}} \bigg|_{st} \cdot \frac{M_{O_2}}{M_B} = \frac{\nu'_{O_2} M_{O_2}}{\nu'_B M_B} \equiv \nu \]
*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:**

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

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: \( Y_{O2,2} \)

- Two-stream system before combustion:
  Divide \( m_{B,u} = Y_{B,1} m_1 \) for stream 1 by total mass

  → Mixture fraction linear with fuel mass

  \[
  Y_{B,u} = Y_{B,1} Z
  \]

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

- Insert into 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:
  \[ \Rightarrow \text{The first two terms in the numerator have to cancel out} \]

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

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

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

• Changes in elements

$$\frac{dn_C}{m\nu_F} = \frac{dn_H}{n\nu_F} = \frac{dn_O}{2\nu_{O_2}}$$

or in terms of element mass fraction

$$\frac{dZ_C}{\nu_F m W_C} = \frac{dZ_H}{\nu_F n W_H} = \frac{dZ_O}{\nu_{O_2} W_{O_2}}$$

• Coupling function:

$$\beta = \frac{Z_C}{\nu_F m W_C} + \frac{Z_H}{\nu_F n W_H} - 2 \frac{Z_O}{\nu_{O_2} W_{O_2}}$$

$\rightarrow \beta$ should not change by chemical reactions
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

$$Z = \frac{Z_C/(mW_C) + Z_H/(nW_H) + 2(Y_{O_2,u} - Z_0)/\left(\nu'_{O_2} W_{O_2}\right)}{Z_{C,1}/(nW_C) + Z_{H,1}/(mW_H) + 2Y_{O_2,u}/\left(\nu'_{O_2} W_{O_2}\right)}$$

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

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

do not change
Relation of mixture fraction with equivalence ratio

- Fuel-air equivalence ratio

\[ \phi = \frac{Y_{F,u}/Y_{O2,u}}{(Y_{F,u}/Y_{O2,u})_{st}} = \frac{\nu Y_{F,u}}{Y_{O2,u}} \]

- Introducing

\[ Y_{F,u} = Y_{F,1}Z \quad \text{and} \quad Y_{O2,u} = Y_{O2,2}(1 - Z) \]

into

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

leads with

\[ \frac{\nu Y_{F,1}}{Y_{O2,2}} = \frac{1 - Z_{st}}{Z_{st}} \]

so 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: $Z_{H,F} = n W_H / W, \quad Z_{C,F} = m W_C / W$
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
• FlameMaster flame calculator

• Definitions, equation of state, mass balance
• Elementary and Global Reactions
• Coupling Functions
• Stoichiometry
• Mixture Fraction
• Burke-Schumann Solution
Burke-Schumann Solution

Diffusion Flame Structure at Complete Conversion

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

  \[ Y_{O_2,b} = Y_{O_2,2} \left(1 - \frac{Z}{Z_{st}}\right), \quad Z \leq Z_{st} \]
Diffusion Flame Structure at Complete Conversion

- 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

$$Y_{F,b} = Y_{F,1} \frac{Z - Z_{st}}{1 - Z_{st}}, \quad Z \geq Z_{st}$$
Diffusion Flame Structure at Complete Conversion

- 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, these 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 $Z = \frac{\nu Y_F - Y_{O_2} + Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}}$ for $Z \geq Z_{st}$

to piecewise linear relations of the product mass fractions in terms of $Z$: 

$Z \leq Z_{st}$: 

$Y_{CO_2,b} = Y_{CO_2,st} \frac{Z}{Z_{st}}$, 

$Y_{H_2O,b} = Y_{H_2O,st} \frac{Z}{Z_{st}}$

$Z \geq Z_{st}$: 

$Y_{CO_2,b} = Y_{CO_2,st} \frac{1 - Z}{1 - Z_{st}}$, 

$Y_{H_2O,b} = Y_{H_2O,st} \frac{1 - Z}{1 - Z_{st}}$

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

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