Combustion Theory and Applications in CFD

CEFRC Combustion Summer School

2014

Prof. Dr.-Ing. Heinz Pitsch

Institut für Technische Verbrennung

RWTH AACHEN UNIVERSITY

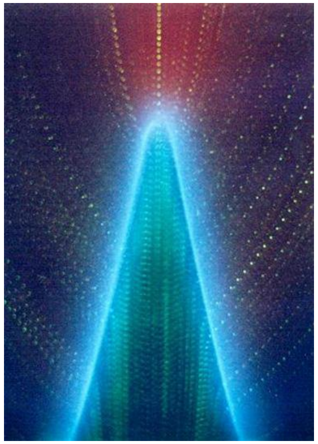
What is Combustion?

- 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

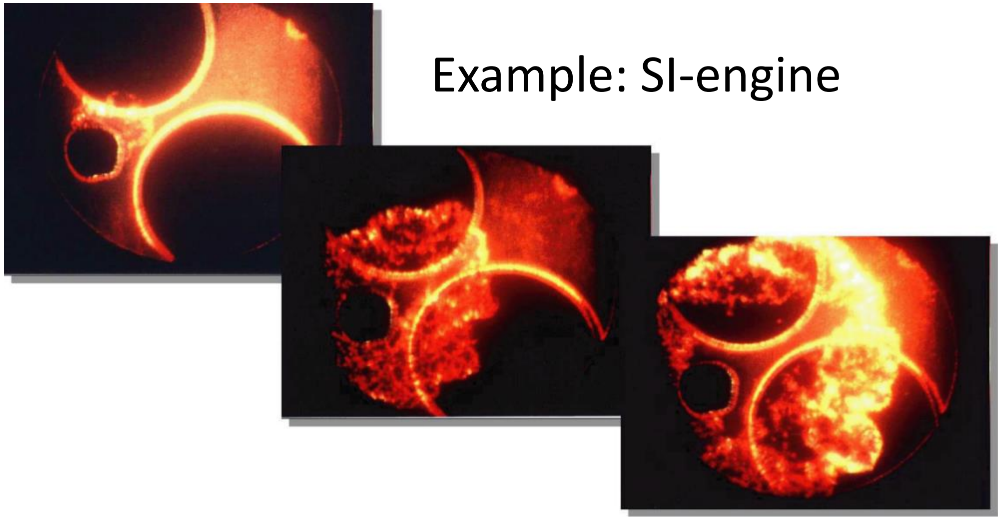
- Important
  - Each chemical or physical process has associated time scale

- Interaction of flow (transport) and chemistry
  - Laminar and turbulent combustion
  - New dimensionless groups (similar to Reynolds number)
    - Damköhler number, Karlovitz number, …



Combustion Applications: Examples

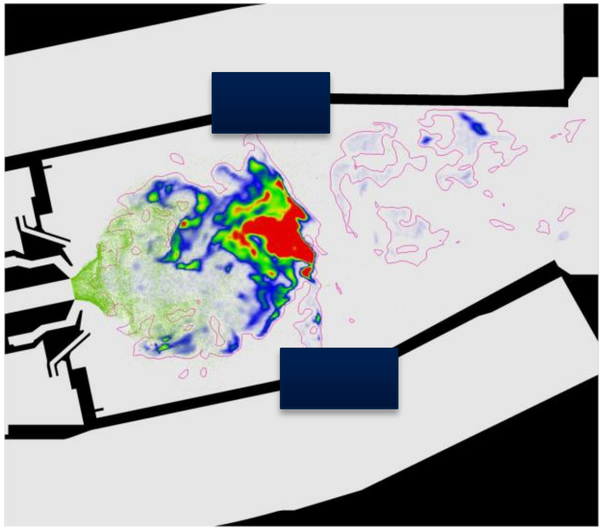
- Premixed combustion
  - Spark-ignition engine
  - Premixed



Example: SI-engine

- Non-premixed combustion
  - Diesel engine
  - Aircraft engine

Example: Aircraft engine



Impact of Combustion

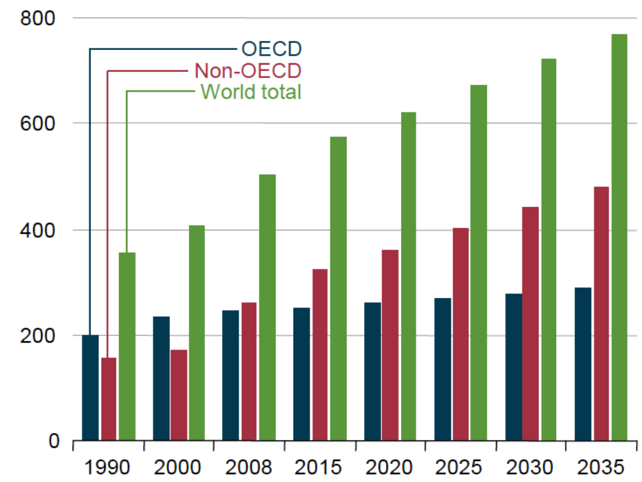
Demand for energy:

- Transport and electricity
- Atmospheric pollution
- Global warming

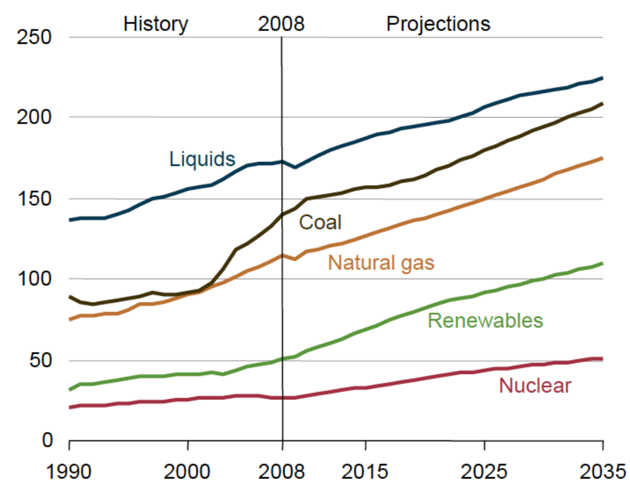
DOE's International Energy Outlook 2011

- 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%

World Energy Consumption [10^{15} Btu]

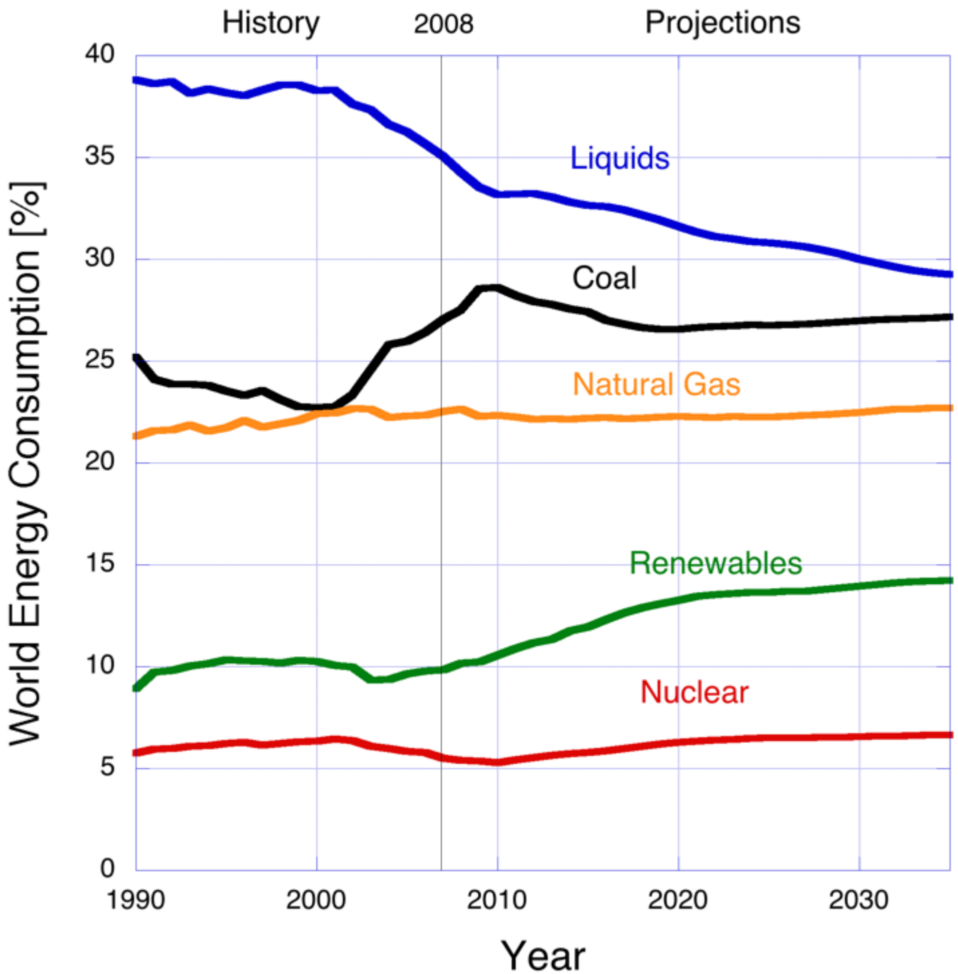


World Energy Consumption by Fuel [10^{15} Btu]



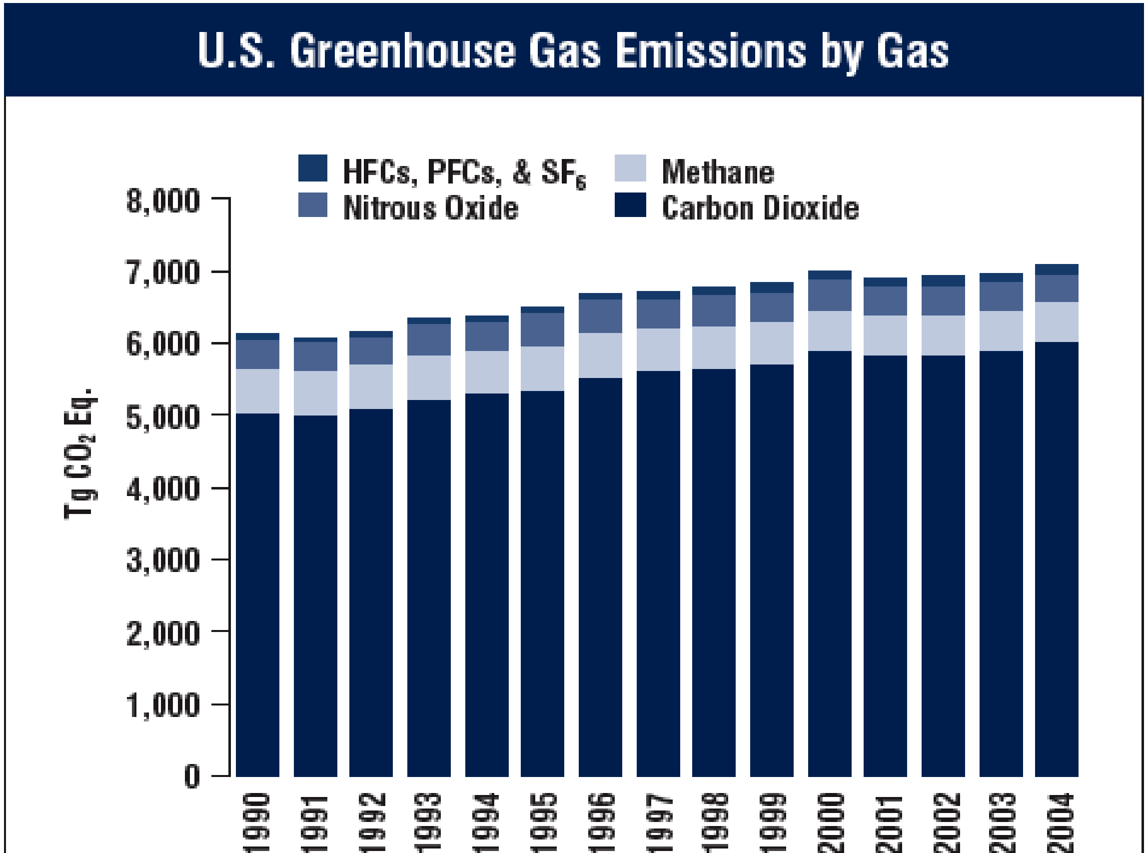
DOE's International Energy Outlook 2011

- 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 CO_2



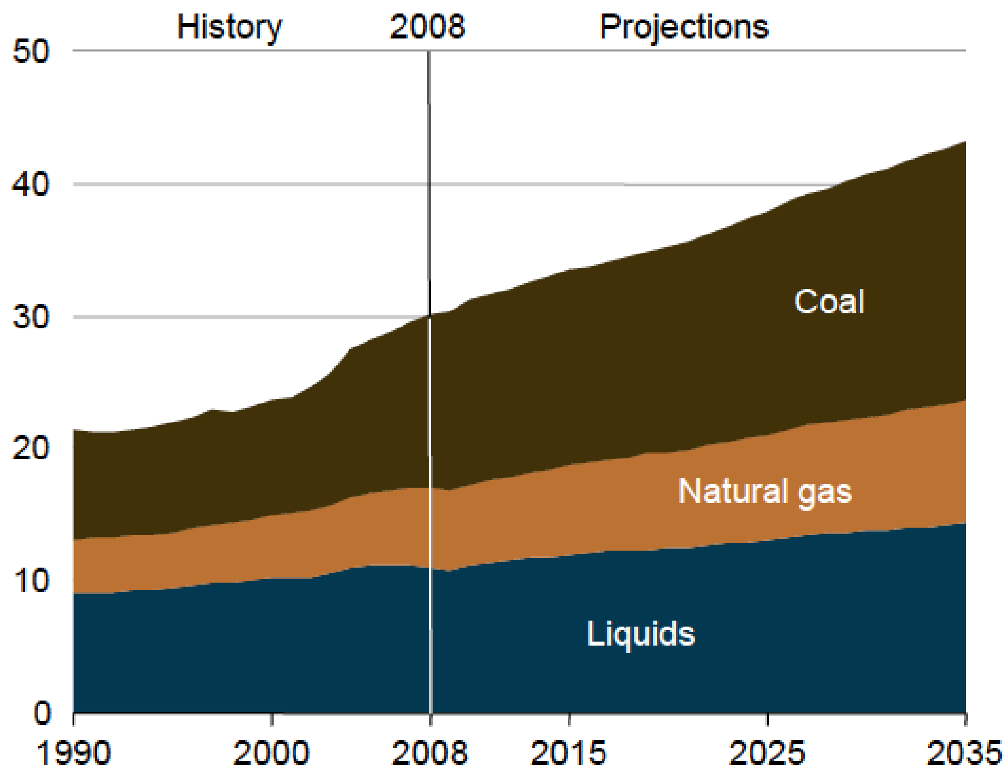
EPA Inventory of US Greenhouse Gas Emissions, 2006

Sources of CO_2

Combustion of fossil fuels:

- 95% of CO_2- emissions
- 80% of all greenhouse gas-emissions
- Expected increase of CO_2 emissions: 43% from 2008 until 2035

World Energy-Related CO_2 Emissions [billion tons]



Quelle: International Energy Outlook, 2011

Reduction of Greenhouse Gas Emissions

Various approaches:

- Hydrogen economy
- CO_2-sequestration (Carbon Capture and Storage, CCS)
- Bio-fuels
- …

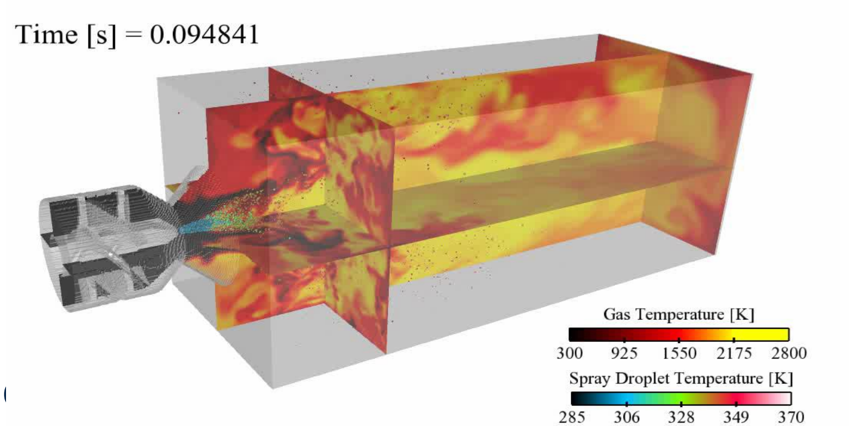
  - Increase in efficiency

⇒ 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 (
    - Flameless oxidation (FLOX) / MILD combustion
- Progress in technology increasingly supported by numerical simulations
- New technologies often lead to changes in operating range

NASA Lean Direct Injection Aircraft Engine Combustor



→ 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^{th} - July 2^{nd}, 2010

Norbert Peters[1]

RWTH Aachen University

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Part I: Fundamentals and Laminar Flames

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- 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

itv Institut für Technische Verbrennung

RWTH AACHEN UNIVERSITY

Thermodynamics

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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→

- Definitions, Equation of State, Mass Balance
- Elementary and Global Reactions
- Coupling Functions
- 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 → 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*: $X_i \equiv \frac{n_i}{n_s}, \quad i = 1, 2, \ldots, k$

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:* $$W = \sum_{i=1}^{k} W_i X_i = [\sum_{i=1}^{k} \frac{Y_i}{W_i}]^{-1}$$

- 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

- 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

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

- 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

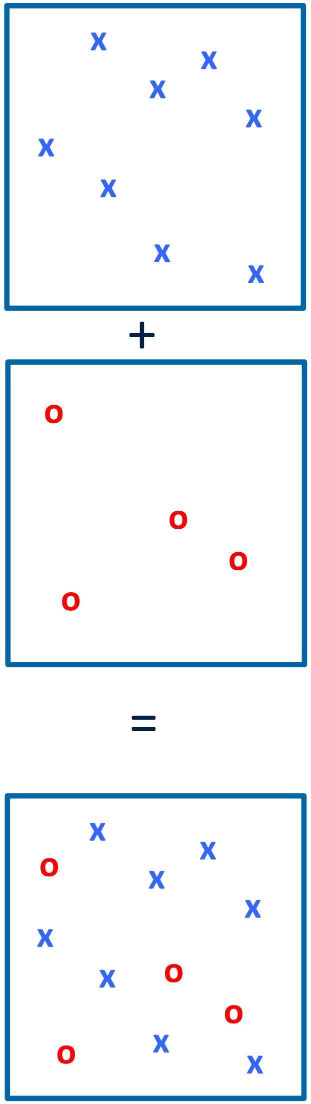
$$p = \sum_{i=1}^{k} p_i = n_s \frac{\mathcal{R}T}{V} = \frac{\rho \mathcal{R}T}{W}$$

- From this follows

$$p_i = p X_i, \quad i = 1, 2, \ldots, k$$

- And for the volume

$$V = n_i \frac{\mathcal{R}T}{p_i} = n \frac{\mathcal{R}T}{p}$$



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: $M_{O_2} \approx 32\ \mathrm{g/mol}\,,\ M_{N_2} \approx 28\ \mathrm{g/mol}\,,\ M_{CH_4} \approx 16\ \mathrm{g/mol}$
  - 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: $Y_{O_2} = 0{,}95\, Y_{O_2,L} = 0{,}22, \quad Y_{N_2} = 0{,}95\, Y_{N_2,L} = 0{,}73$
  - Mean molar mass: $M = [\sum_{i=1}^{3} Y_i/M_i]^{-1} = 27{,}5\ \mathrm{g/mol}$

Example: Methane/Air Mixture

- Mole fractions of Components: $X_i = M/M_i\, Y_i$

$$X_{\mathrm{CH_4}} = 0,09,\ X_{\mathrm{O_2}} = 0,19\,,\ X_{\mathrm{N_2}} = 0,72$$

- Molar mass of elements: $M_{\mathrm{H}} \approx 1\ \mathrm{g/mol}, \quad M_{\mathrm{C}} \approx 12\ \mathrm{g/mol}$

- with: $$Z_j = \sum_{i=1}^{3} \frac{a_{ij}\, M_j}{M_i}\, Y_i$$

- Mass fractions of elements: $Z_{\mathrm{H}} = 0,0125, \quad Z_{\mathrm{C}} = 0,0375, \quad Z_{\mathrm{O}} = Y_{\mathrm{O_2}}, \quad Z_{\mathrm{N}} = Y_{\mathrm{N_2}}$

- 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 $$H^\circ + O_2 \rightarrow OH^\circ + O^\circ$$
  - Only take place, if collisions between reactants take place
  - Reaction velocities can be determined experimentally oder theoretically

- Global reactions
  - Conversion of educts to products $$2H_2 + O_2 = 2H_2O$$
  - Ratios of amounts of substance
  - Does not represent a chemical micro-process
  - Temporal process of the reaction cannot be given

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

$$H^\circ + O_2 \rightarrow OH^\circ + O^\circ$$

- Elementary reactions also proceed backwards:

$$H^\circ + O_2 \leftarrow OH^\circ + O^\circ$$

- Often symbolized by a double arrow:

$$H^\circ + O_2 \rightleftharpoons OH^\circ + O^\circ$$

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: $$2H_2 + O_2 = 2H_2O$$

  meaning that 2 mol H_2 react with 1 mol O_2, yielding 2 mol H_2O

Global reactions

- Multiples of the equation are also valid:

$$H_2 + \frac{1}{2}O_2 = H_2O$$

  – This does not hold for elementary reactions!

- Multiplication of the equation of the global reaction by the molar masses

  → Mass balance during combustion

- Example: Combustion of H_2 using the foregoing equation

$$2\,g\,H_2 + 16\,g\,O_2 = 18\,g\,H_2O$$

Global reactions

- Stoichiometric coefficient of reactants *i*: ν_i'
- Stoichiometric coefficient of products *i*: ν_i''
- Stoichiometric coefficient of a component (only for global reactions): $\nu_i := \nu_i'' - \nu_i'$
- Note:
  - Stoichiometric coefficients ν_i of the educts are negative!
  - Whereas ν_i' are defined to be positive!

Global reactions

Formulation of global reactions:

- Combustion of hydrocarbon fuel or an alcohol

$$\nu'_B B + \nu'_{O_2} O_2 = \nu''_{CO_2} CO_2 + \nu''_{H_2O} H_2O$$

- 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 ν_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

Global reaction, e.g.: ν_1 F + ν_2 O = ν_3 P

- Conversion of:
  - n_1 moles of component 1
  - n_i moles of component *i*

- Reaction has taken place n_1/ν_1 or n_i/ν_i times → $n_1/\nu_1 = n_i/\nu_i$
- 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 → Coupling function:

$$\frac{Y_{\mathrm{O_2}} - Y_{\mathrm{O_2},u}}{\nu'_{\mathrm{O_2}} M_{\mathrm{O_2}}} = \frac{Y_{\mathrm{B}} - Y_{\mathrm{B},u}}{\nu'_{\mathrm{B}} M_{\mathrm{B}}}$$

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Stoichiometry

- Stoichiometric:
  - Fuel-to-oxygen ratio such that both are entirely consumed when combustion to CO_2 and H_2O is completed

- For example,
  - Global reaction describing combustion of a single component hydrocarbon fuel C_mH_n (subscript F for fuel)

$$\nu'_{\mathrm{F}}\mathrm{C}_m\mathrm{H}_n + \nu'_{\mathrm{O_2}}\mathrm{O_2} = \nu''_{\mathrm{CO_2}}\mathrm{CO_2} + \nu''_{\mathrm{H_2O}}\mathrm{H_2O}$$

  - Stoichiometric coefficients are

$$\nu'_{\mathrm{F}} = 1,\;\; \nu'_{\mathrm{O_2}} = m + \frac{n}{4},\;\; \nu''_{\mathrm{CO_2}} = m \;\; \nu''_{\mathrm{H_2O}} = \frac{n}{2}$$

where $\nu'_{\mathrm{F}} = 1$ may be chosen arbitrarily to unity

Stoichiometric Mass Ratio

- Mole number ratio for stoichiometric condition

$$\frac{n_{O_2,u}}{n_{F,u}}\Big|_{st} = \frac{\nu'_{O_2}}{\nu'_F}$$

or in terms of mass fractions

$$\frac{Y_{O_2,u}}{Y_{F,u}}\Big|_{st} = \frac{\nu'_{O_2} W_{O_2}}{\nu'_F W_F} = \nu$$

where ν is called the stoichiometric mass ratio

- Typical value: Methane: $\nu = 4$
- Mass ratio ν

→ Fuel and oxidizer are both consumed when combustion is completed

Stoichiometric Mass Ratio

- This is consistent with coupling function, since

$$\frac{Y_{\mathrm{O}_2} - Y_{\mathrm{O}_2,u}}{\nu'_{\mathrm{O}_2} W_{\mathrm{O}_2}} = \frac{Y_{\mathrm{F}} - Y_{\mathrm{F},u}}{\nu'_{\mathrm{F}} W_{\mathrm{F}}}$$

leads to

$$\nu Y_F - Y_{\mathrm{O}_2} = \nu Y_{\mathrm{F},u} - Y_{\mathrm{O}_2,u}$$

- Complete consumption of fuel and oxygen

$$Y_{\mathrm{F}} = Y_{\mathrm{O}_2} = 0$$

leads to

$$\frac{Y_{\mathrm{O}_2,u}}{Y_{\mathrm{F},u}} \Big|_{st} = \frac{\nu'_{\mathrm{O}_2} W_{\mathrm{O}_2}}{\nu'_{\mathrm{F}} W_{\mathrm{F}}} = \nu$$

*Extra: Minimum oxygen requirement

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

  → Fuel/air mole number ratio before combustion at stoichiometric conditions

  → Ratio of the stoichiometric coefficients

$$o_{\text{min},m} = \left.\frac{n_{\text{O}_2,u}}{n_{\text{B},u}}\right|_{st} = \left.\frac{X_{\text{O}_2,u}}{X_{\text{B},u}}\right|_{st} = \frac{\nu'_{\text{O}_2}}{\nu'_{\text{B}}}$$

- Minumum oxygen requirement (mass): o_{min}

$$o_{\text{min}} = \left.\frac{m_{\text{O}_2,u}}{m_{\text{B},u}}\right|_{st} = \left.\frac{X_{\text{O}_2,u}}{X_{\text{B},u}}\right|_{st} \cdot \frac{M_{\text{O}_2}}{M_{\text{B}}} = \frac{\nu'_{\text{O}_2} M_{\text{O}_2}}{\nu'_{\text{B}} M_{\text{B}}} \equiv \nu$$

*Extra: Minimum air requirement

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

$$\ell_{\mathrm{min}}$$

- Relation between minimum oxygen and minimum air requirement:

$$\ell_{\mathrm{min}} = \frac{o_{\mathrm{min}}}{Y_{\mathrm{O_2,Luft}}}, \quad \ell_{\mathrm{min},m} = \frac{o_{\mathrm{min},m}}{X_{\mathrm{O_2,Luft}}} \Rightarrow \ell_{\mathrm{min}} = \frac{o_{\mathrm{min}}}{0,232}, \quad \ell_{\mathrm{min},m} = \frac{o_{\mathrm{min},m}}{0,21}$$

with:

- Mass fraction $Y_{O2,air} = 0{,}232$
- Mole fraction $X_{O2,air} = 0{,}21$

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

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

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

- Stoichiometric mass ratio ν 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

Note: Index B means fuel

- 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 $m_{B,u} = Y_{\mathrm{B},1} m_1$ by the total mass flow, yields

→ Mixture fraction linear with fuel mass

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

$$Y_{\mathrm{O}_2,u} = Y_{\mathrm{O}_2,2}\,(1 - Z)$$

➢ Coupling function: $\nu Y_{\mathrm{B}} - Y_{\mathrm{O}_2} = \nu Y_{\mathrm{B},u} - Y_{\mathrm{O}_2,u}$

$$Z = \frac{\nu Y_{\mathrm{B}} - Y_{\mathrm{O}_2} + Y_{\mathrm{O}_2,2}}{\nu Y_{\mathrm{B},1} + Y_{\mathrm{O}_2,2}}$$

The mixture fraction

- Mixture fraction: $$Z = \frac{\nu Y_{\mathrm{B}} - Y_{\mathrm{O}_2} + Y_{\mathrm{O}_2,2}}{\nu Y_{\mathrm{B},1} + Y_{\mathrm{O}_2,2}}$$

- For stoichiometric composition:
  → The first two terms in the numerator have to cancel out

➢ Stoichiometric mixture fraction:

$$Z_{st} = \frac{Y_{\mathrm{O}_2,2}}{\nu Y_{\mathrm{F},1} + Y_{\mathrm{O}_2,2}}$$

$$Z_{st} = [1 + \nu \frac{Y_{\mathrm{B},1}}{Y_{\mathrm{O}_2,2}}]^{-1} = [1 + \frac{\nu'_{\mathrm{O}_2} M_{\mathrm{O}_2} Y_{\mathrm{B},1}}{\nu'_{\mathrm{B}} M_{\mathrm{B}} Y_{\mathrm{O}_2,2}}]^{-1}$$

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:

$$\beta = \frac{Z_C}{\nu'_F m W_C} + \frac{Z_H}{\nu'_F n W_H} - 2\frac{Z_O}{\nu'_{O_2} W_{O_2}}$$

→ Changes in β 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

$$Z = \frac{Z_\mathrm{C}/(mW_\mathrm{C}) + Z_\mathrm{H}/(nW_\mathrm{H}) + 2(Y_{\mathrm{O}_2,u} - Z_\mathrm{O})/(\nu'_{\mathrm{O}_2} W_{\mathrm{O}_2})}{Z_{\mathrm{C},1}/(nW_\mathrm{C}) + Z_{\mathrm{H},1}/(mW_\mathrm{H}) + 2Y_{\mathrm{O}_2,u}/(\nu'_{\mathrm{O}_2} W_{\mathrm{O}_2})}$$

- 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

$$\phi = \frac{Y_{\mathsf{F},u}/Y_{\mathsf{O}_2,u}}{(Y_{\mathsf{F},u}/Y_{\mathsf{O}_2,u})_{st}} = \frac{\nu Y_{\mathsf{F},u}}{Y_{\mathsf{O}_2,u}}$$

- Introducing $Y_{\mathsf{F},u} = Y_{\mathsf{F},1} Z$ and $Y_{\mathsf{O}_2,u} = Y_{\mathsf{O}_2,2}(1-Z)$

into $\nu Y_F - Y_{\mathsf{O}_2} = \nu Y_{\mathsf{F},u} - Y_{\mathsf{O}_2,u}$

leads with $\dfrac{\nu Y_{\mathsf{F},1}}{Y_{\mathsf{O}_2,2}} = \dfrac{1-Z_{st}}{Z_{st}}$

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

$$\phi = \frac{Z}{1-Z} \frac{(1-Z_{st})}{Z_{st}}$$

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:

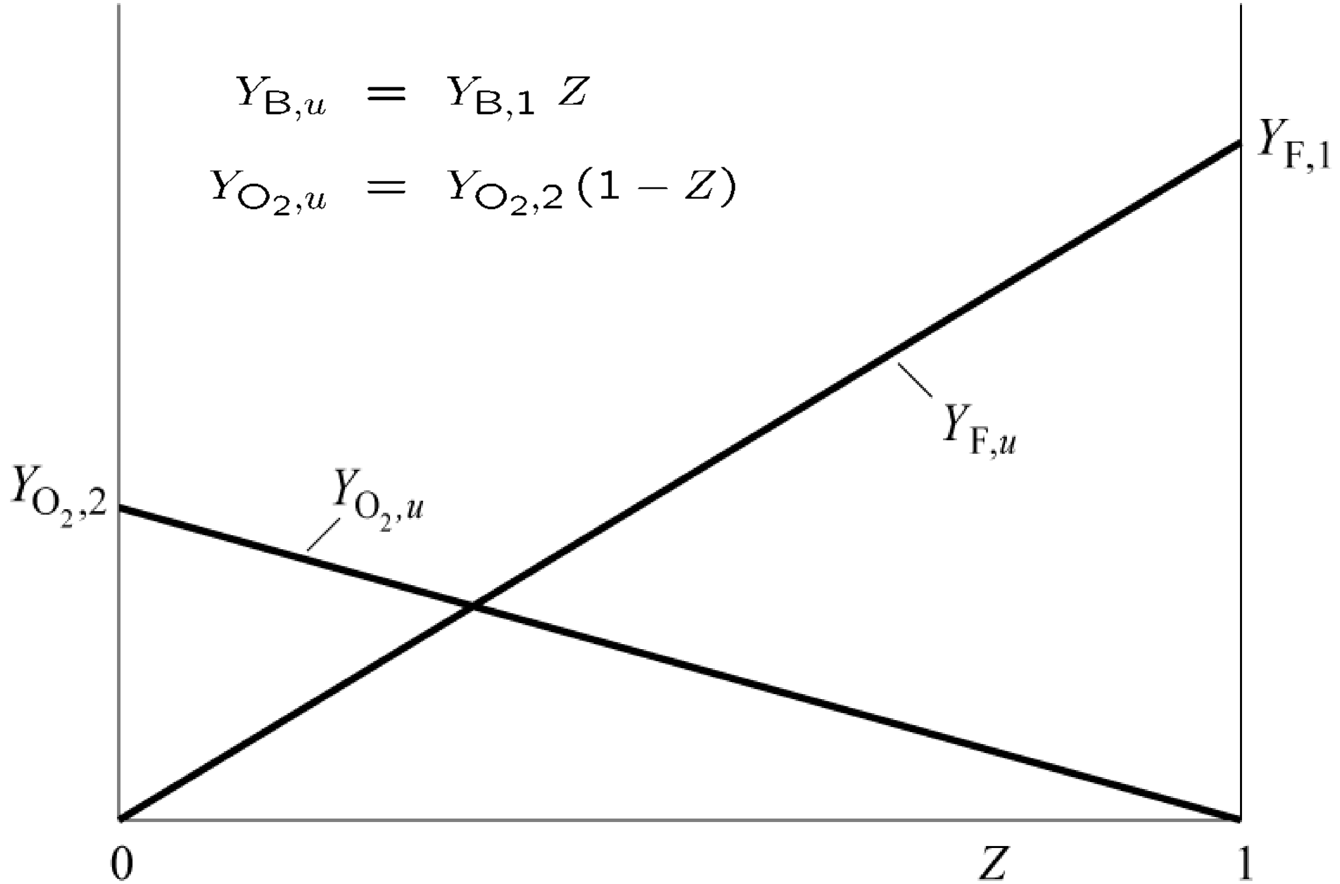
- The element mass fractions $Z_{\mathrm{H,F}}, Z_{\mathrm{C,F}}$ of a mixture of hydrocarbons and its mean molecular weight W are assumed to be known
- Determine its stoichiometric mixture fraction in air
- Hint: $Z_{\mathrm{H,F}} = n\,W_{\mathrm{H}}/W\,, \quad Z_{\mathrm{C,F}} = m\,W_{\mathrm{C}}/W$

Diffusion Flame Structure at Complete Conversion

Profiles of Y_F and Y_{O_2} in the unburnt gas

unburnt mixture

$$Y_{B,u} = Y_{B,1}\, Z$$
$$Y_{O_2,u} = Y_{O_2,2}\,(1 - Z)$$



Diffusion Flame Structure at Complete Conversion

- Stoichiometric composition

$$Z_{st} = \frac{Y_{\mathrm{O}_2,2}}{\nu Y_{\mathrm{F},1} + Y_{\mathrm{O}_2,2}}$$

- If $Z < Z_{st}$, fuel is deficient
  - Mixture is fuel lean
  - Combustion terminates when all fuel is consumed: $Y_{\mathrm{F},b} = 0$

    (burnt gas, subscript *b*)

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

$$Z = \frac{\nu Y_{\mathrm{F}} - Y_{\mathrm{O}_2} + Y_{\mathrm{O}_2,2}}{\nu Y_{\mathrm{F},1} + Y_{\mathrm{O}_2,2}}$$

as

$$Y_{\mathrm{O}_2,b} = Y_{\mathrm{O}_2,2}(1 - \frac{Z}{Z_{st}}), \quad Z \leq Z_{st}$$

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

$$Z_{\mathrm{C}} = m\frac{W_{\mathrm{C}}}{W_{\mathrm{F}}}Y_{\mathrm{F},u}, \quad Z_{\mathrm{H}} = n\frac{W_{\mathrm{H}}}{W_{\mathrm{F}}}Y_{\mathrm{F},u}, \quad Z_{\mathrm{O}} = Y_{\mathrm{O}_2,u}$$

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

$$Z_{\mathrm{C}} = m\frac{W_{\mathrm{C}}}{W_{\mathrm{F}}}Y_{\mathrm{F},b} + \frac{W_{\mathrm{C}}}{W_{\mathrm{CO}_2}}Y_{\mathrm{CO}_2,b}$$

$$Z_{\mathrm{H}} = n\frac{W_{\mathrm{H}}}{W_{\mathrm{F}}}Y_{\mathrm{F},b} + 2\frac{W_{\mathrm{H}}}{W_{\mathrm{H}_2\mathrm{O}}}Y_{\mathrm{H}_2\mathrm{O},b}$$

$$Z_{\mathrm{O}} = 2\frac{W_{\mathrm{O}}}{W_{\mathrm{O}_2}}Y_{\mathrm{O}_2,b} + 2\frac{W_{\mathrm{O}}}{W_{\mathrm{CO}_2}}Y_{\mathrm{CO}_2,b} + \frac{W_{\mathrm{O}}}{W_{\mathrm{H}_2\mathrm{O}}}Y_{\mathrm{H}_2\mathrm{O},b}$$

- Elements are conserved, hence $Z_{j,u} = Z_{j,b}$

Diffusion Flame Structure at Complete Conversion

- This leads with $Y_{\mathrm{F},u} = Y_{\mathrm{F},1} Z$ and $Y_{\mathrm{F},b} = 0$ for $Z \leq Z_{st}$

  and $Z = \dfrac{\nu Y_\mathrm{F} - Y_{\mathrm{O}_2} + Y_{\mathrm{O}_2,2}}{\nu Y_{\mathrm{F},1} + Y_{\mathrm{O}_2,2}}$ for $Z \geq Z_{st}$

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

$$Z \leq Z_{st}: \quad Y_{\mathrm{CO}_2,b} = Y_{\mathrm{CO}_2,st} \frac{Z}{Z_{st}} \quad Y_{\mathrm{H}_2\mathrm{O},b} = Y_{\mathrm{H}_2\mathrm{O},st} \frac{Z}{Z_{st}}$$

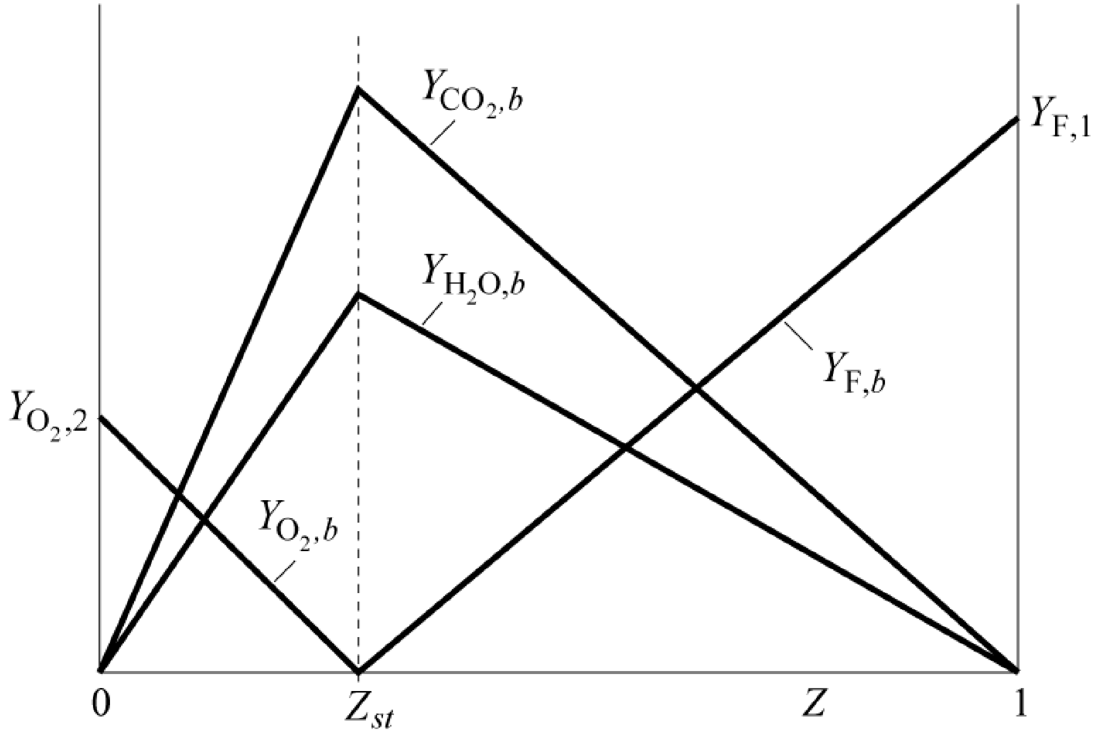
$$Z \geq Z_{st}: \quad Y_{\mathrm{CO}_2,b} = Y_{\mathrm{CO}_2,st} \frac{1-Z}{1-Z_{st}}, \quad Y_{\mathrm{H}_2\mathrm{O},b} = Y_{\mathrm{H}_2\mathrm{O},st} \frac{1-Z}{1-Z_{st}}$$

  where

$$Y_{\mathrm{CO}_2,st} = Y_{\mathrm{F},1} Z_{st} \frac{m W_{\mathrm{CO}_2}}{W_\mathrm{F}}$$

Diffusion Flame Structure at Complete Conversion

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