

Combustion Theory and Applications in CFD

Princeton Combustion Summer School
2018

Prof. Dr.-Ing. Heinz Pitsch



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Combustion Applications

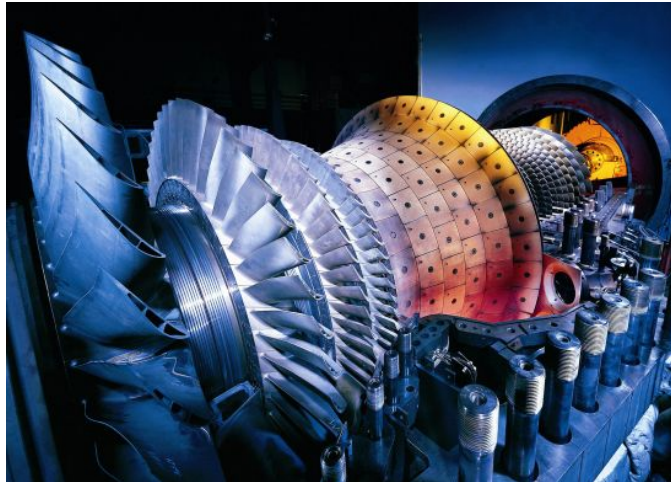


Mobility & Transport



Combustion Applications

Power Generation

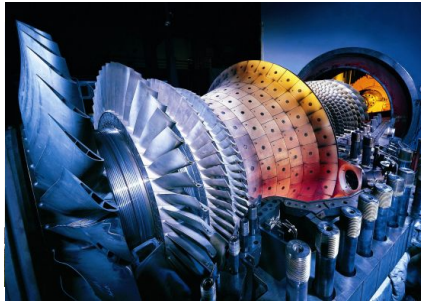


Mobility & Transport

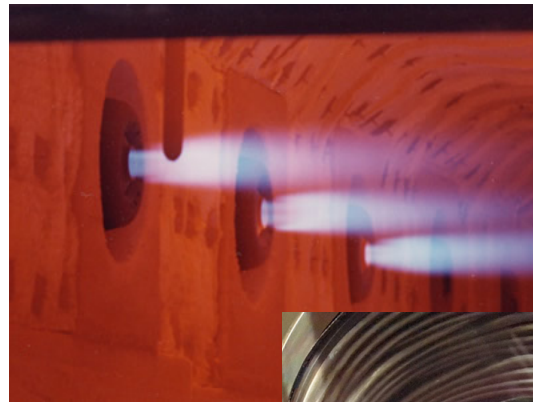


Combustion Applications

Power Generation



Industry & Household

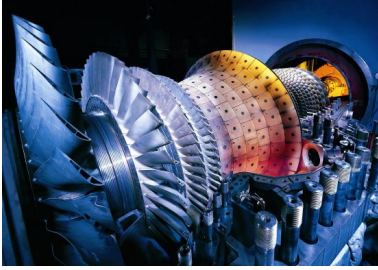


Mobility & Transport

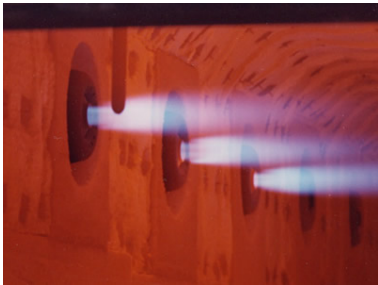


Combustion Applications

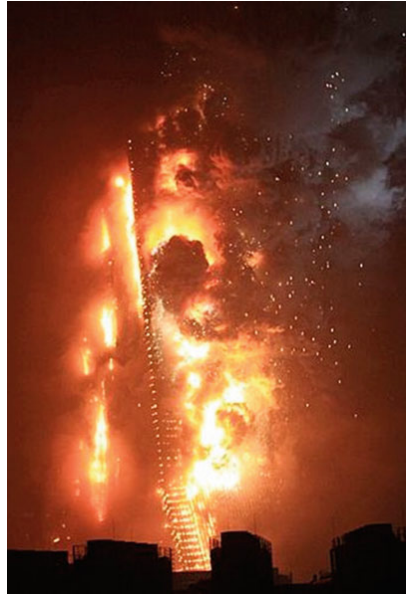
Power Generation



Industry & Household



Fire Safety & Explosions



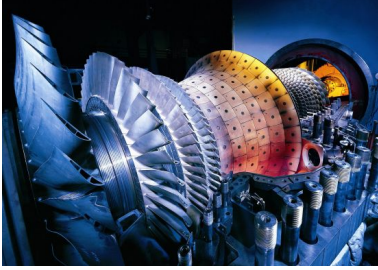
NIST: Safe Refrigerants

Mobility & Transport

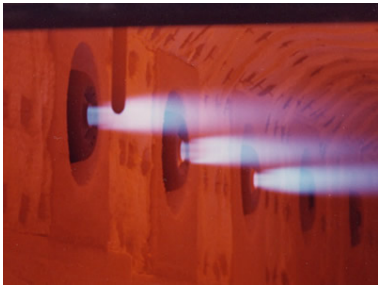


Combustion Applications

Power Generation



Industry & Household



Combustion is omnipresent!

But causes emissions of

- Harmful pollutants
- Greenhouse gases

Design challenge

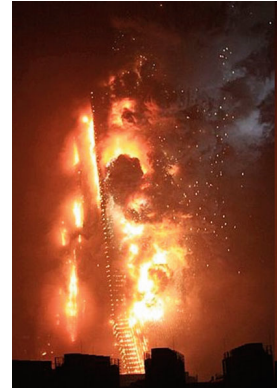
- Combustion extremely complex, multi-scale & multi-physics
- Devices usually big and high power
- Measurement in severe environments difficult

➔ Computational engineering
very important

Mobility & Transport



Fire Safety & Explosions



Combustion Science

- Combustion research started many years ago



- Why is combustion science still **important**?
- Why is combustion science **interesting**?
- HPC as an important step

US DOE's International Energy Outlook 2016

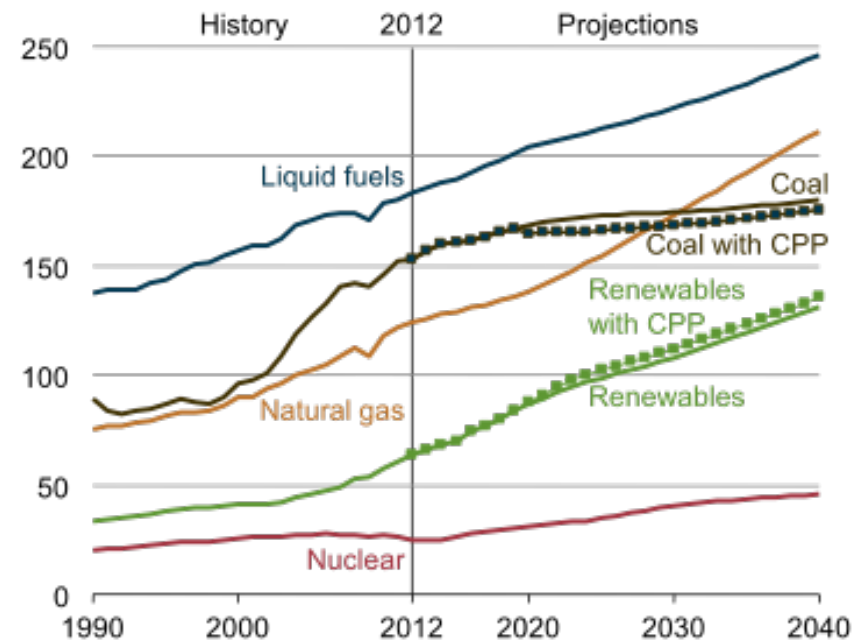
World Energy Consumption

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

Large numbers

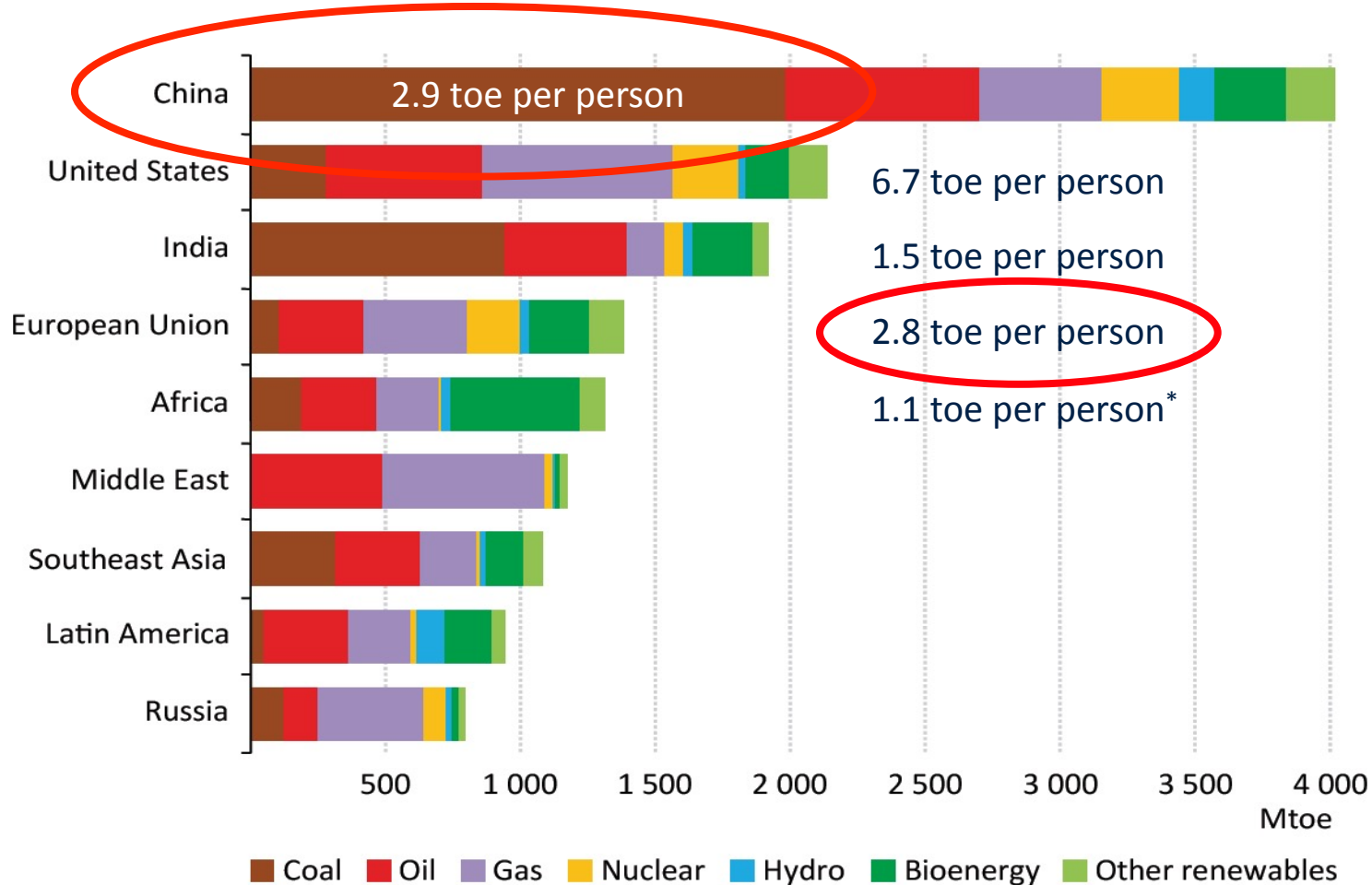
- 120 million tons daily CO₂ emissions in 2040
 - ➔ 13 kg daily per person
- 10 billion liter daily fuel consumption
 - ➔ 1.3 liter daily liquid fuel use

World Energy Consumption by Fuel [10¹⁵ Btu]

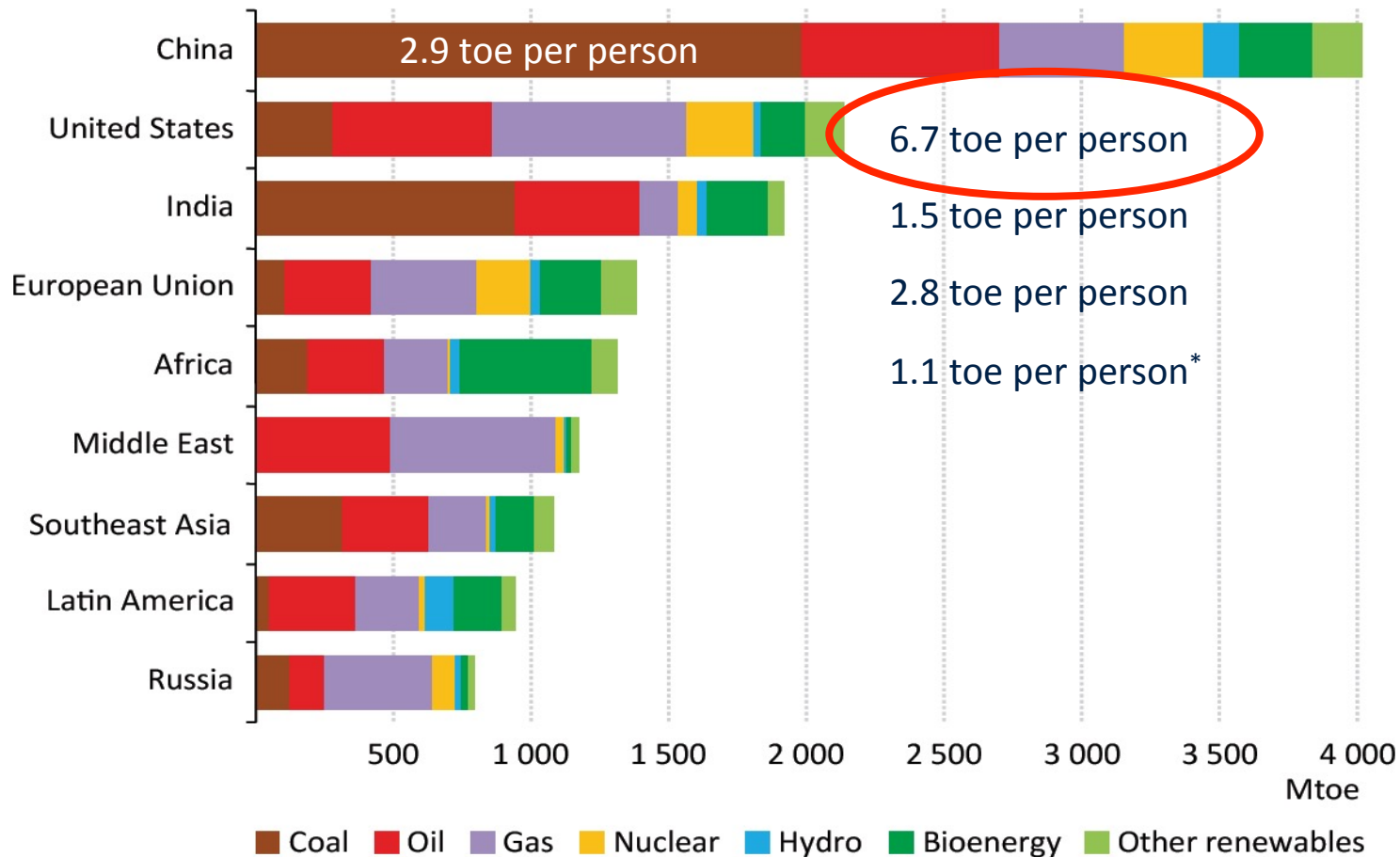


Clean combustion extremely important!

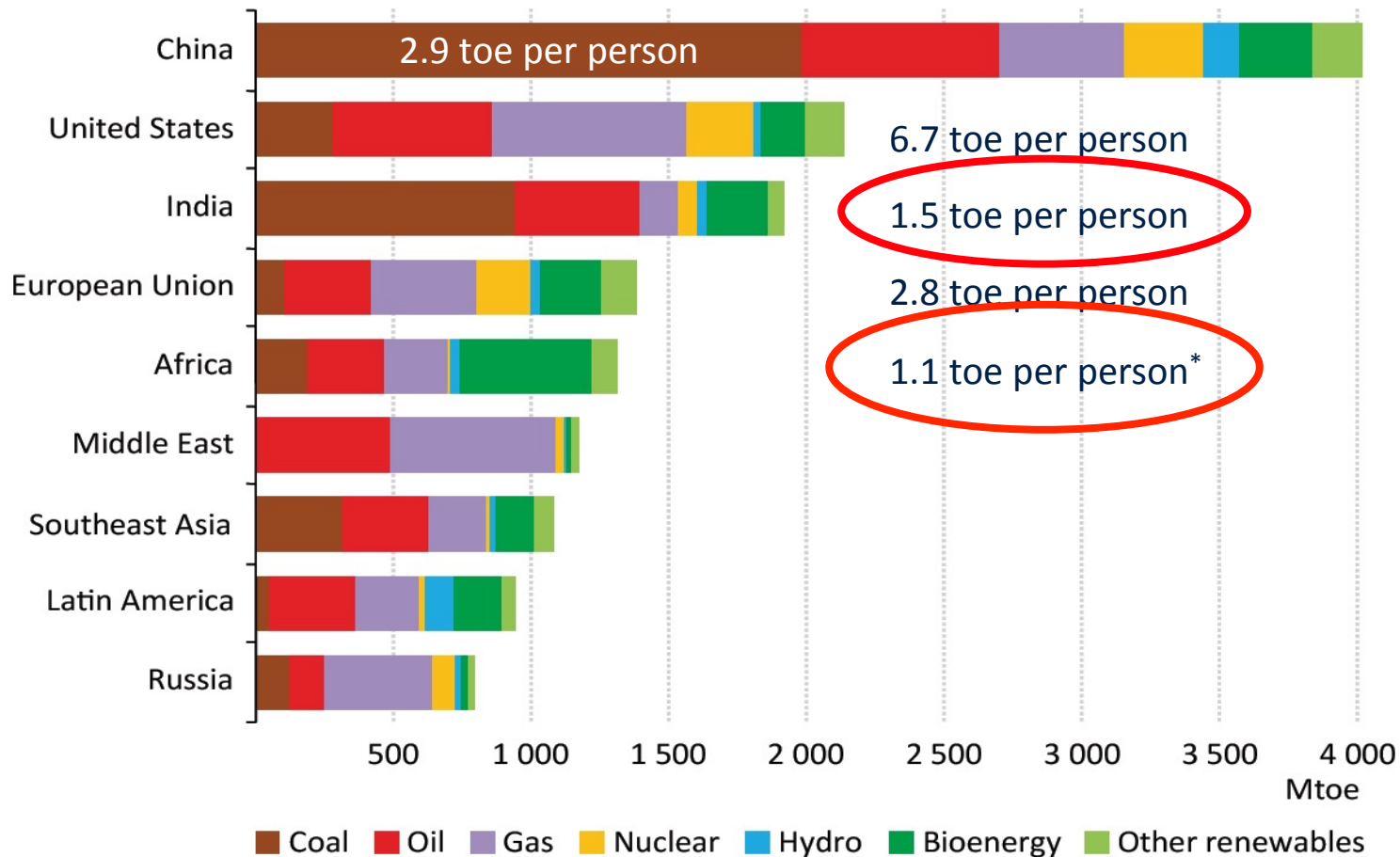
Primary Energy Demand by Region & Source in 2040



Primary Energy Demand by Region & Source in 2040



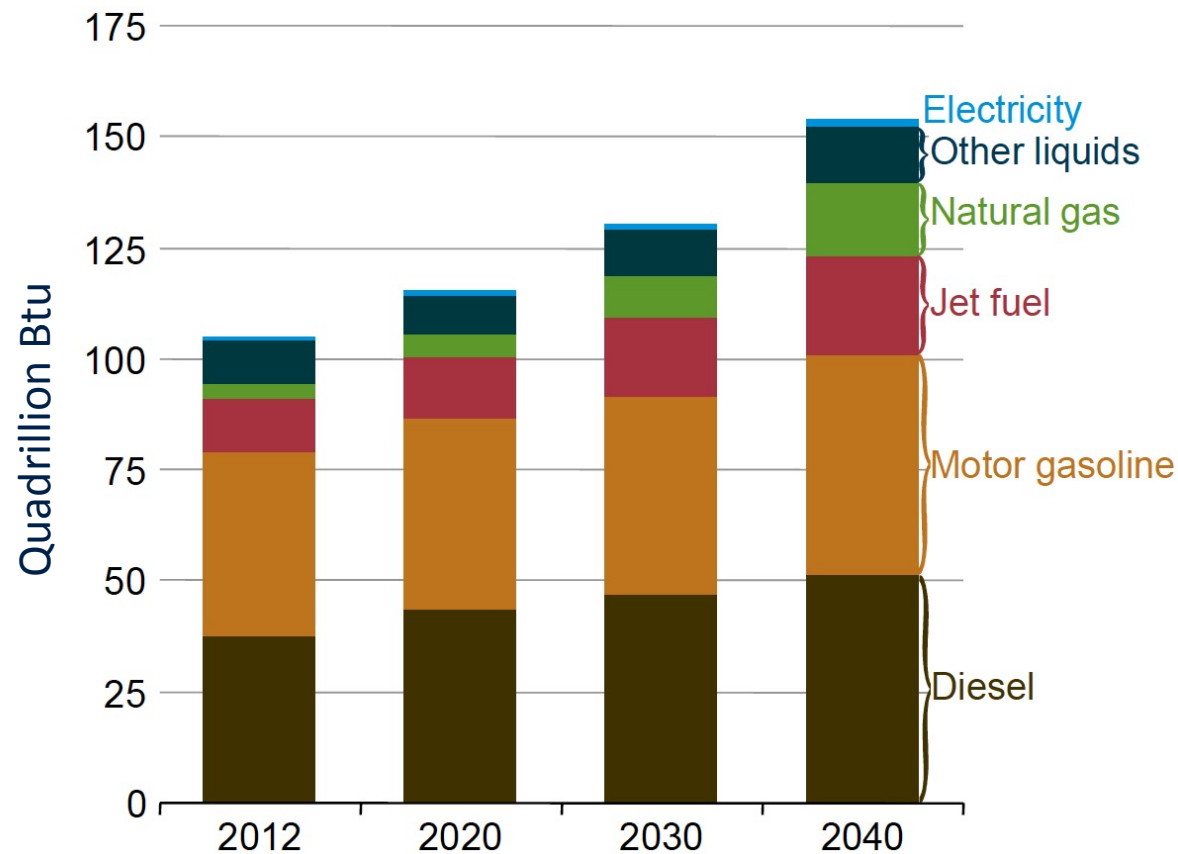
Primary Energy Demand by Region & Source in 2040



Transport Sector World Energy Consumption by Source

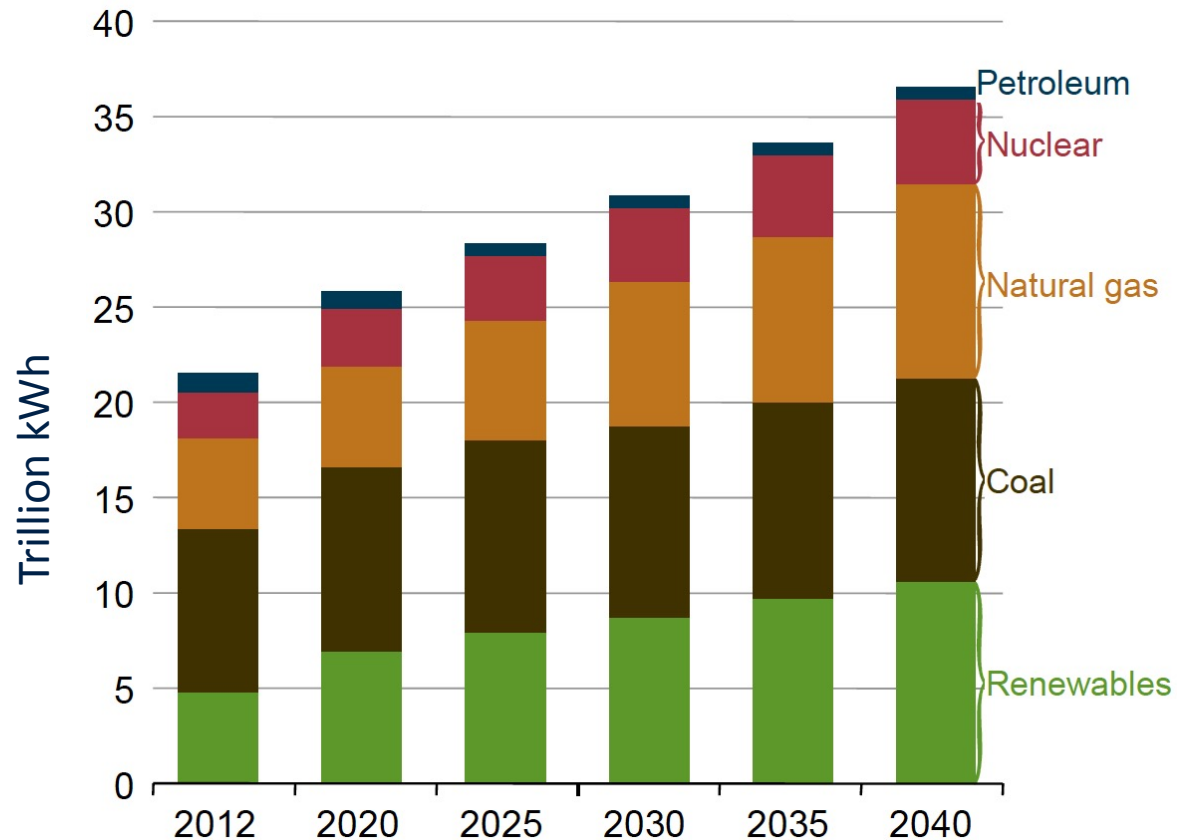
- Fraction of Battery Electric Vehicle (BEV) in 2040 still small

➔ 6% BEV for 450 scenario



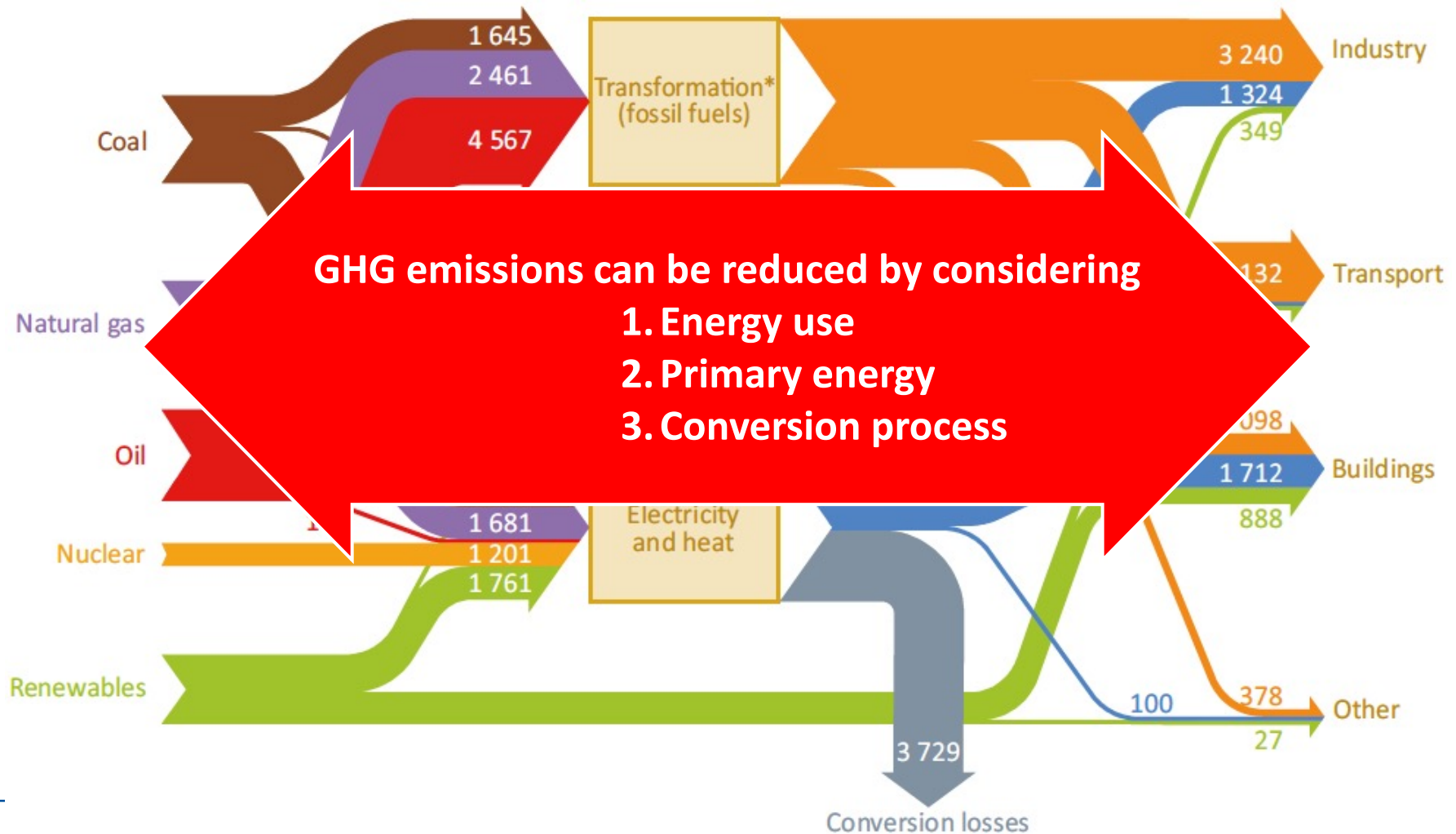
World Net Electricity Generation by Source

- For positive effect of BEV, electric power should be from renewable sources



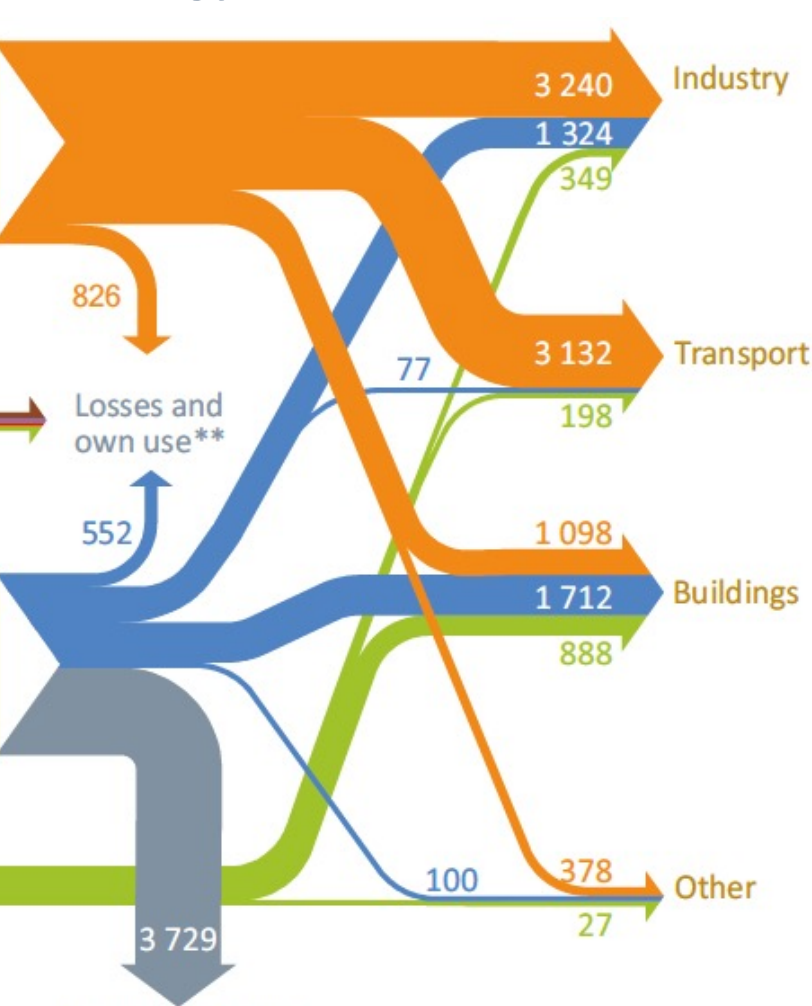
IEA's World Energy Outlook 2015

World Energy Demand in Mtoe by Fuel & Sector in 2040



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
 - ...

Conversion losses

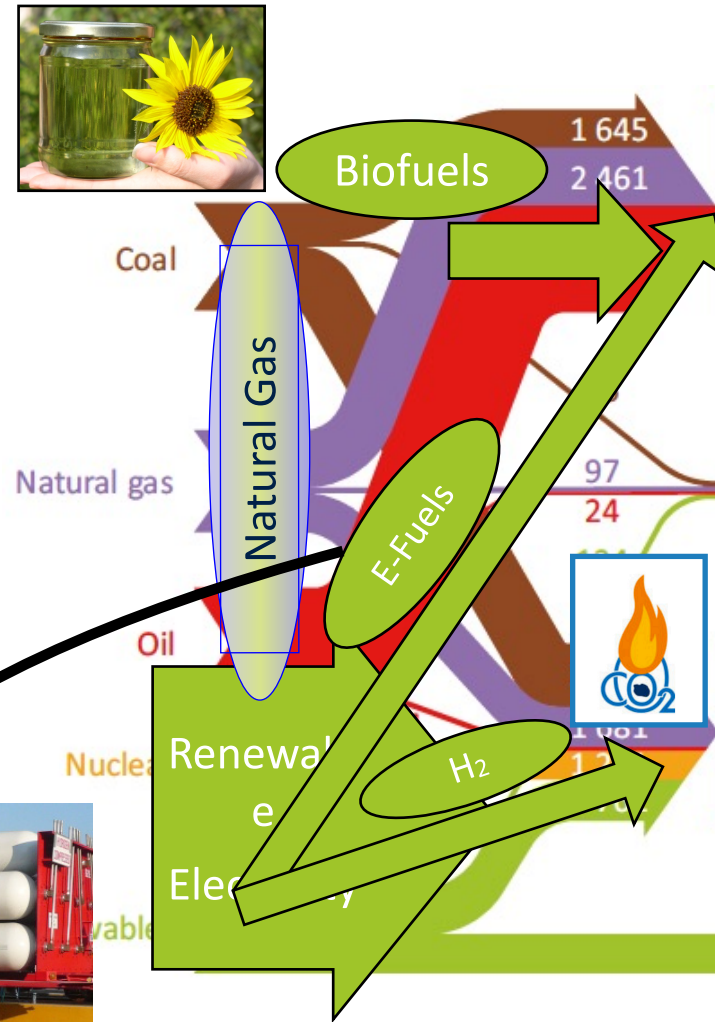
Institute for Combustion Technology | Heinz Pitsch

Mitigation of GHG Emissions

Primary Energy and Conversion Process

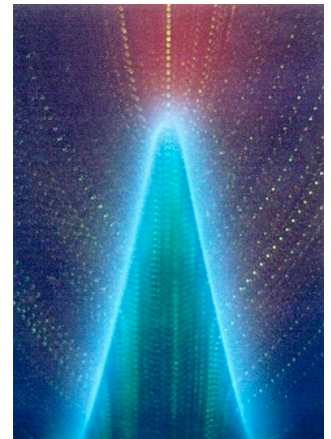
Opportunities

- 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



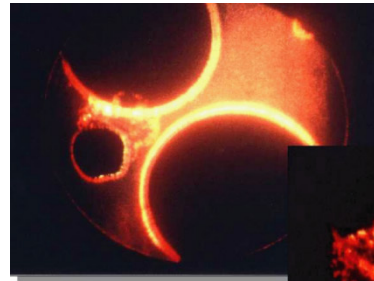
What is Combustion?

- 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, ...

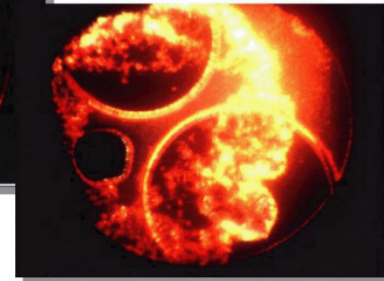
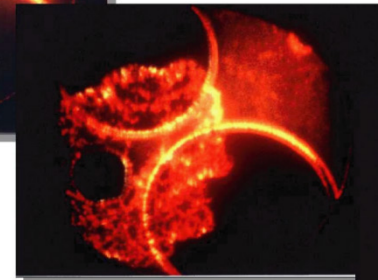


Combustion Applications: Examples

- Premixed combustion
 - Spark-ignition engine
 - Premixed

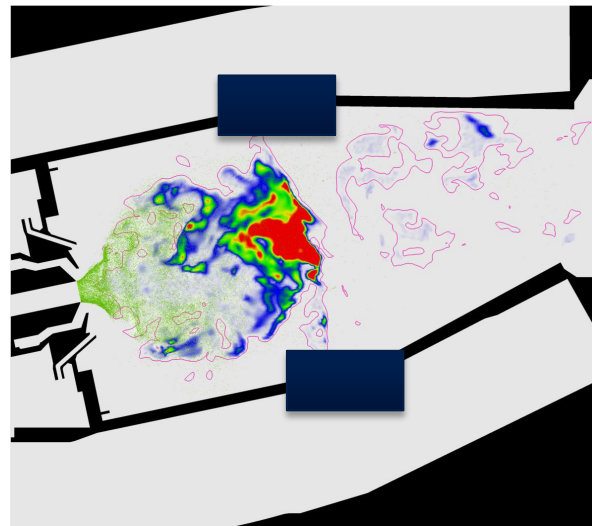


Example: SI-engine



- Non-premixed combustion
 - Diesel engine
 - Aircraft engine

Example: Aircraft engine



Various approaches:

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



Combustion Theory

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

Part I: Fundamentals and Laminar Flames

Part II: Turbulent Combustion

Combustion Theory

CEFRC Summer School

Princeton


June 28th - July 2nd, 2010

Norbert Peters¹

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

Fundamentals and Mass Balances of Combustion Systems

Princeton Combustion Summer School
2018

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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- Definitions, Equation of State, Mass Balance
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- Coupling Functions
- 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 : $X_i \equiv \frac{n_i}{n_s}, \quad i = 1, 2, \dots, k$

The mass fraction

- Mass m_i of all molecules of species i is related to its number of moles by

$$m_i = W_i n_i, \quad i = 1, 2, \dots, k$$

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 : $Y_i = \frac{m_i}{m}, \quad i = 1, 2, \dots, k$

- 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:

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

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

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

- 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:

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

- 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

$$\rho = \frac{m}{V}, \quad \rho_i = \frac{m_i}{V} = \rho Y_i, \quad i = 1, 2, \dots, k$$

- Partial molar density is related to partial density and mass fraction by

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

(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**

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

- 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

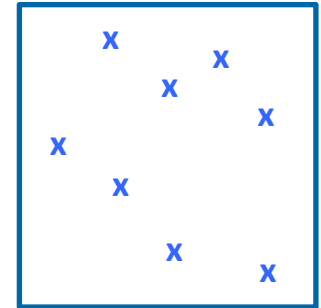
$$p = \sum_{i=1}^k p_i = n_s \frac{\mathcal{R}T}{V} = \frac{\rho \mathcal{R}T}{W}$$

- From this follows

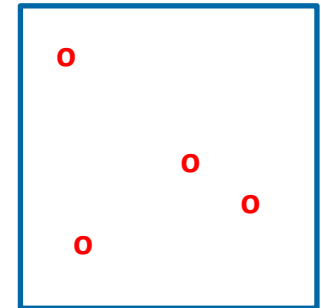
$$p_i = pX_i, \quad i = 1, 2, \dots, k$$

- And for the volume

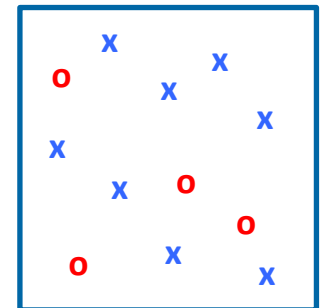
$$V = n_i \frac{\mathcal{R}T}{p_i} = n \frac{\mathcal{R}T}{p}$$



+



=



*Example: Methane/Air Mixture

- Known: 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: $Y_{O_2} = 0,95 Y_{O_2,L} = 0,22, \quad Y_{N_2} = 0,95 Y_{N_2,L} = 0,73$

- Mean molar mass: $M = \left[\sum_{i=1}^3 Y_i / M_i \right]^{-1} = 27,5 \text{ g/mol}$

*Example: Methane/Air Mixture

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

$$X_{\text{CH}_4} = 0,09, \quad X_{\text{O}_2} = 0,19, \quad X_{\text{N}_2} = 0,72$$


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

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

- Mass fractions of elements: $Z_{\text{H}} = 0,0125, \quad Z_{\text{C}} = 0,0375, \quad Z_{\text{O}} = Y_{\text{O}_2}, \quad Z_{\text{N}} = Y_{\text{N}_2}$
- Simplification: Whole numbers for values of the molar masses

Course Overview

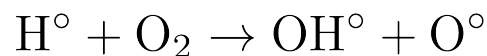
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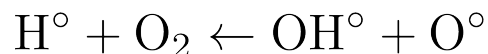
- Distinction between elementary reactions and global reactions **important!**
- Elementary reactions
 - Describe actual micro-process of chemical reaction
$$\text{H}^\circ + \text{O}_2 \rightarrow \text{OH}^\circ + \text{O}^\circ$$
 - Only take place, if collisions between reactants take place
 - Reaction velocities can be determined experimentally oder theoretically
- Global reactions
 - Conversion of educts to products
$$2\text{H}_2 + \text{O}_2 = 2\text{H}_2\text{O}$$
 - Ratios of amounts of substance
 - Does **not** represent a chemical micro-process
 - Temporal process of the reaction cannot be given

Elementary Reactions

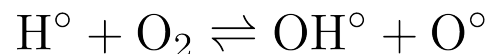
- Observe the conservation of elements
- Chemical changes due to collisions of components
- Transition from educts to products symbolized by arrow
- Example: Bimolecular elementary reaction



- Elementary reactions also proceed backwards:



- Often symbolized by a double arrow:



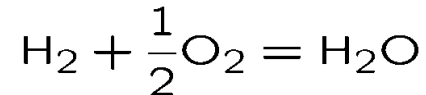
Global reactions

- 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: $2\text{H}_2 + \text{O}_2 = 2\text{H}_2\text{O}$

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:



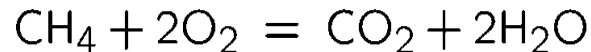
– This does not hold for elementary reactions!

- 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



Global reactions

- Stoichiometric coefficient of reactants i : ν_i'
- Stoichiometric coefficient of products i : ν_i''
- Example:



$$- \nu_{\text{CH}_4}' = 1, \quad \nu_{\text{H}_2\text{O}}'' = 2$$

- **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 ν_i of reactants are negative!
- ν_i' are defined to be positive!

Global reactions

Formulation of global reactions:

- Combustion of hydrocarbon fuel or an alcohol



- Atoms in the fuel: Carbon, hydrogen and oxygen
 - Number of atoms in the fuel a_{BC} , a_{BH} , a_{BO}
- Stoichiometric coefficients of the global reaction are derived from ν'_B
 - Balances of atoms

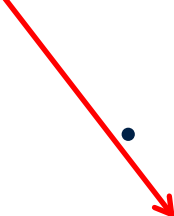
- C: $\nu''_{CO_2} = a_{BC} \nu'_B$
- H: $\nu''_{H_2O} = a_{BH} \nu'_B / 2$
- O: $\nu'_{O_2} = \nu''_{CO_2} + \nu''_{H_2O} / 2 - a_{BO} \nu'_B / 2$

- 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

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:

$$\frac{dC_i}{dt} = \nu_i \omega \quad \text{with} \quad C_i = n_i/V$$

or

$$\frac{dn_i/\nu_i}{dt} = \omega V$$

→ Change of n_i/ν_i same for all species

Coupling functions

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/ν_1 or n_i/ν_i times $\rightarrow n_1/\nu_1 = n_i/\nu_i$
- Differential notation:

$$\frac{dn_i}{\nu_i} = \frac{dn_1}{\nu_1}, \quad \frac{dm_i}{\nu_i M_i} = \frac{dm_1}{\nu_1 M_1}, \quad \frac{dY_i}{\nu_i M_i} = \frac{dY_1}{\nu_1 M_1} \quad (i = 1, 2, \dots, n)$$

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

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

Coupling functions – Example H₂

Coupling function:

$$\frac{Y_{O_2} - Y_{O_2,u}}{\nu'_{O_2} M_{O_2}} = \frac{Y_B - Y_{B,u}}{\nu'_B M_B} \quad \Leftrightarrow \quad \Delta Y_{O_2} = \underbrace{\nu}_{\nu = \frac{\nu'_{O_2} M_{O_2}}{\nu'_B M_B}} \Delta Y_B$$

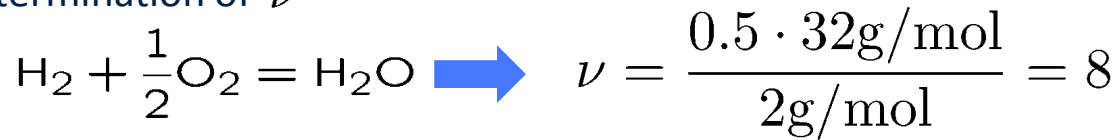
Example:

A closed system contains H₂ and 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 ν



$$\Delta m_{O_2} = 8 \cdot 1 \text{kg} = 8 \text{kg}$$

→ For burning 1kg H₂, 8kg × 76.7/23.3 = 26.3 kg of air is needed

Coupling functions – Example Gasoline

Example: How much CO₂ 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 $\text{I-C}_8\text{H}_{18} + 12.5 \text{ O}_2 = 8 \text{ CO}_2 + 9 \text{ H}_2\text{O}$

2. Coupling function between fuel and CO₂

$$\frac{dm_B}{\nu'_B M_B} = \frac{dm_{\text{CO}_2}}{\nu''_{\text{CO}_2} M_{\text{CO}_2}}$$

3. Integrations leads to

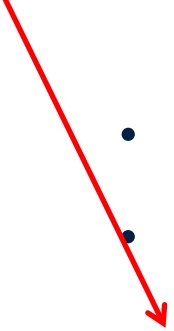
$$\Delta m_{\text{CO}_2} = \frac{\nu''_{\text{CO}_2} M_{\text{CO}_2}}{\nu'_B M_B} \Delta m_B$$

→ During combustion of 1 liter Gasoline, 2.3 kg CO₂ are produced

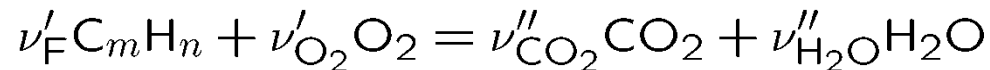
→ Under standard conditions, this is roughly 1.3 m³ CO₂

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- Stoichiometric:
 - **Fuel-to-oxygen ratio** such that both are entirely consumed when combustion to CO₂ and H₂O is completed
- For example,
 - Global reaction describing combustion of a single component hydrocarbon fuel C_mH_n (subscript F for fuel)



- Stoichiometric coefficients are

$$\nu'_F = 1, \quad \nu'_{O_2} = m + \frac{n}{4}, \quad \nu''_{CO_2} = m \quad \nu''_{H_2O} = \frac{n}{2}$$

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

Stoichiometric Mass Ratio

- Mole number ratio for stoichiometric condition

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

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 values: Methane: $\nu = 4$; N-Dodecane: $\nu = 3.5$
- Mass ratio ν
 - Fuel and oxidizer are **both consumed** when combustion is completed

Stoichiometric Mass Ratio

- This is consistent with coupling function, since

$$\frac{Y_{O_2} - Y_{O_2,u}}{\nu'_{O_2} W_{O_2}} = \frac{Y_F - Y_{F,u}}{\nu'_F W_F}$$

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

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

*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

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

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

$$o_{\min} = \frac{m_{O_2,u}}{m_{B,u}} \Big|_{st} = \frac{X_{O_2,u}}{X_{B,u}} \Big|_{st} \cdot \frac{M_{O_2}}{M_B} = \frac{\nu'_{O_2} M_{O_2}}{\nu'_B M_B} \equiv \nu$$

*Extra: Minimum air requirement

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

$$\ell_{\min}$$

- Relation between minimum oxygen and minimum air requirement:

$$\ell_{\min} = \frac{o_{\min}}{Y_{\text{O}_2, \text{Luft}}}, \quad \ell_{\min, m} = \frac{o_{\min, m}}{X_{\text{O}_2, \text{Luft}}} \Rightarrow \ell_{\min} = \frac{o_{\min}}{0,232}, \quad \ell_{\min, m} = \frac{o_{\min, m}}{0,21}$$

with:

- Mass fraction $Y_{\text{O}_2, \text{air}} = 0,232$
- Mole fraction $X_{\text{O}_2, \text{air}} = 0,21$

The equivalence ratio

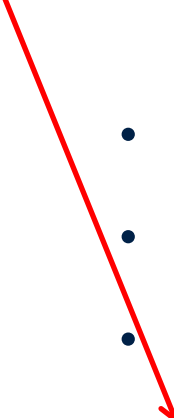
- The **equivalence ratio** is the ratio of fuel to oxidizer ratio in the unburnt to that of a stoichiometric mixture
- For combustion with oxygen

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

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

- Mass fraction of fuel in the fuel stream: $Y_{B,1}$
- Mass fraction of oxygen in the oxidizer stream: $Y_{O_2,2}$

Note: Index B means fuel

- 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

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

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

- Insert into coupling function: $\nu Y_B - Y_{O_2} = \nu Y_{B,u} - Y_{O_2,u}$

$$Z = \frac{\nu Y_B - Y_{O_2} + Y_{O_2,2}}{\nu Y_{B,1} + Y_{O_2,2}}$$

The mixture fraction

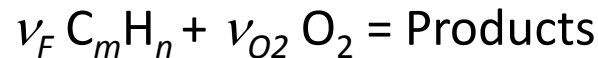
- Mixture fraction:
$$Z = \frac{\nu Y_B - Y_{O_2} + Y_{O_2,2}}{\nu Y_{B,1} + Y_{O_2,2}}$$
- For **stoichiometric** composition:
 - The first two terms in the numerator have to cancel out
- Stoichiometric mixture fraction:

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

$$Z_{st} = \left[1 + \nu \frac{Y_{B,1}}{Y_{O_2,2}} \right]^{-1} = \left[1 + \frac{\nu'_{O_2} M_{O_2} Y_{B,1}}{\nu'_B M_B Y_{O_2,2}} \right]^{-1}$$

Mixture fraction definition by Bilger

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



- 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:

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

→ β 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

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

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

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

do not change

- 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

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

The equivalence ratio

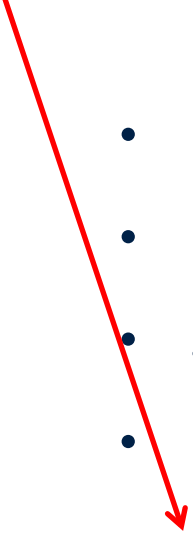
- This relation is also valid for multicomponent fuels (see exercise below)
- It illustrates that the mixture fraction is **simply another expression for the local equivalence ratio**

Exercise:

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

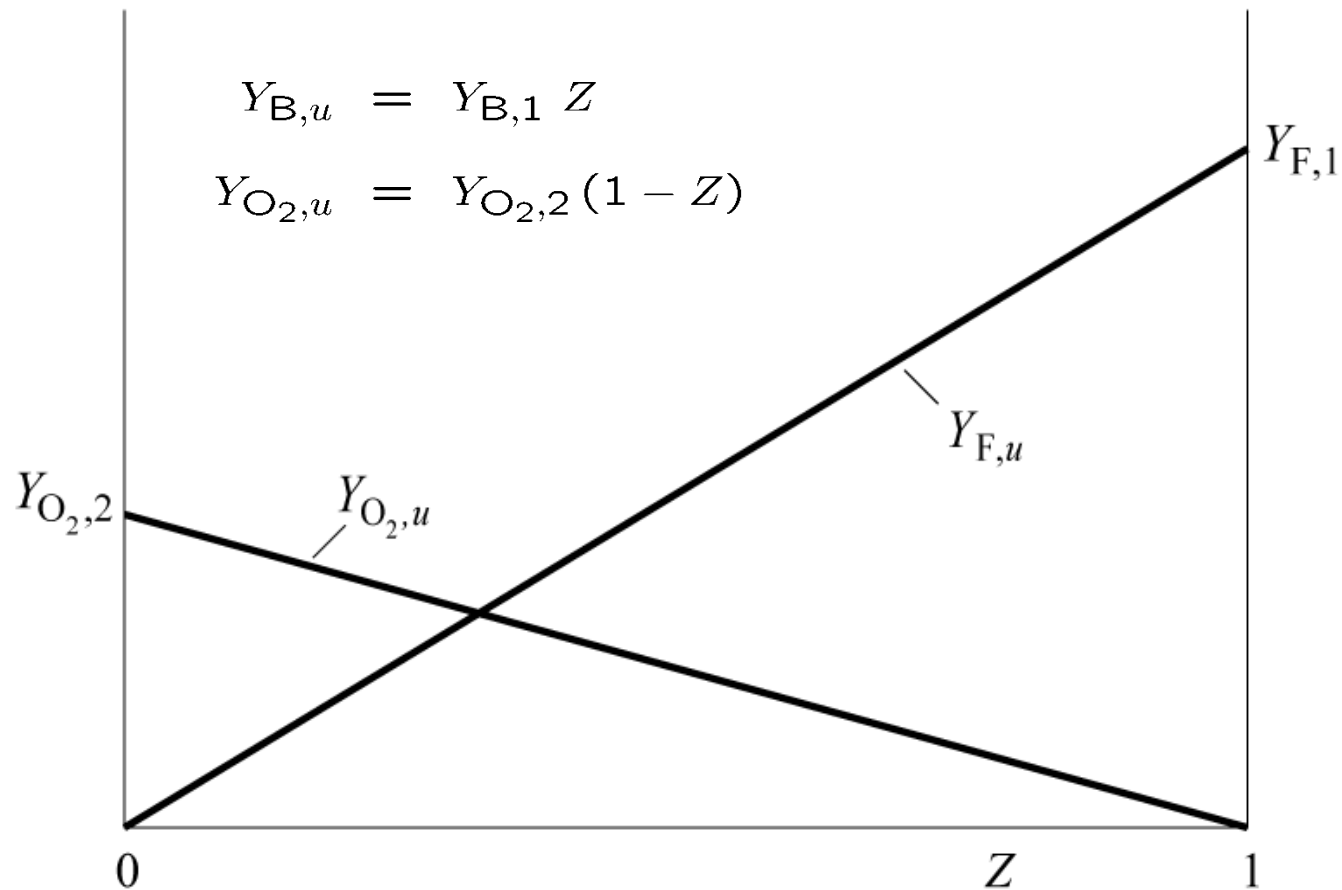
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Diffusion Flame Structure at Complete Conversion

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



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

to [piecewise linear relations](#) of the product mass fractions in terms of Z :

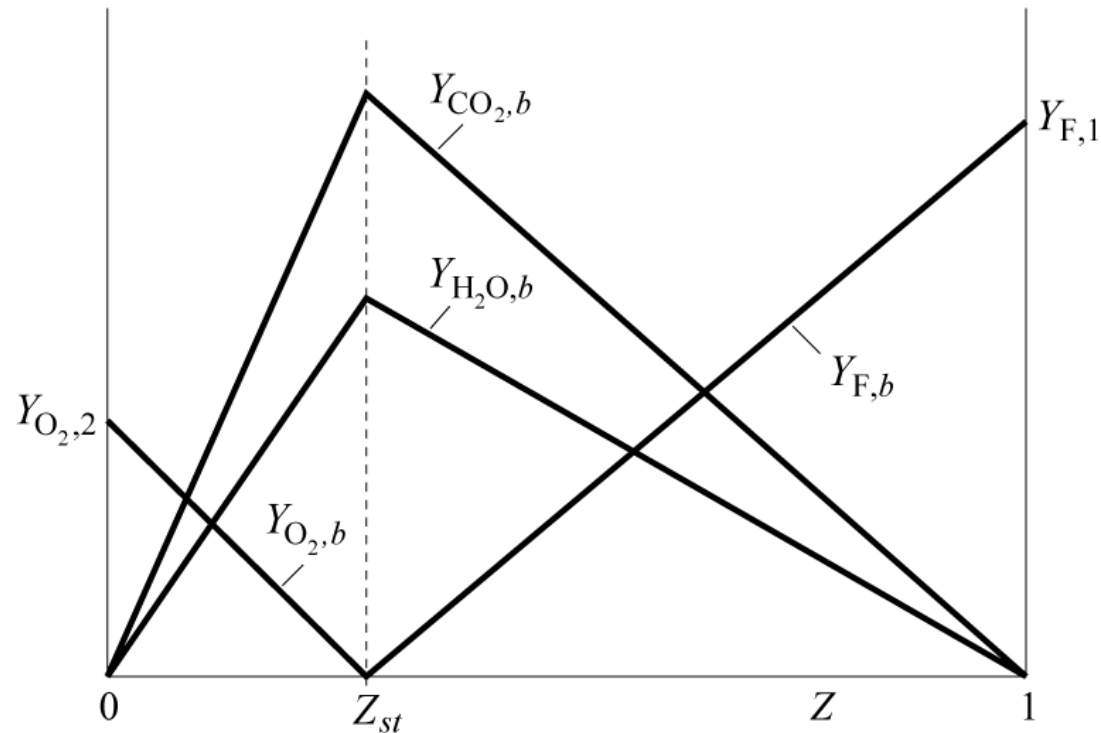
$$Z \leq Z_{st} : \quad Y_{CO_2,b} = Y_{CO_2,st} \frac{Z}{Z_{st}} \quad Y_{H_2O,b} = Y_{H_2O,st} \frac{Z}{Z_{st}}$$

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

where

$$Y_{CO_2,st} = Y_{F,1} Z_{st} \frac{mW_{CO_2}}{W_F}$$

Profiles in the burning mixture



Burke-Schumann Solution:



Infinitely fast, irreversible chemistry

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