4A13
Combustion and Engines
Lent. 2022

Combustion:

Prof. N. Swaminathan (ns341)
Hopkinson Lab – ISG-17

8 = 7L + 1Ex.

Quantitative/qualitative questions

Engines:

Prof. S. Hochgreb (sh372)
Hopkinson Lab

Topics

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1. Basics – multicomp. Mixt. Xi, Yi, stoichio. Govern. Eqs. T_f
2. Chemical equilibrium and kinetics – combustion chemistry
3. Limit reactors – Autoignition & Extinction
4. Laminar Premixed
5. Laminar Non-premixed
6. Pollutants
7. Turbulent flames – Introd. (not examinable)
8. Example Class

Textbooks – Combustion

- I. Glassman, *Combustion, 1996*
- *Spalding Combustion & Mass transfer, 1978*
- S. Turns, *Introduction to Combustion, 2000*

- C. K. Law, *Combustion Physics, 2006*
- *Kuo Principles of Combustion, 1984*
- T. Poinsot & T. Veynante, *Theoretical and Numerical Combustion*

Outline – for Today

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- Why study combustion?
- Stoichiometry and thermochemistry
- Flame temperature
- Conservation equations

Why study Combustion?

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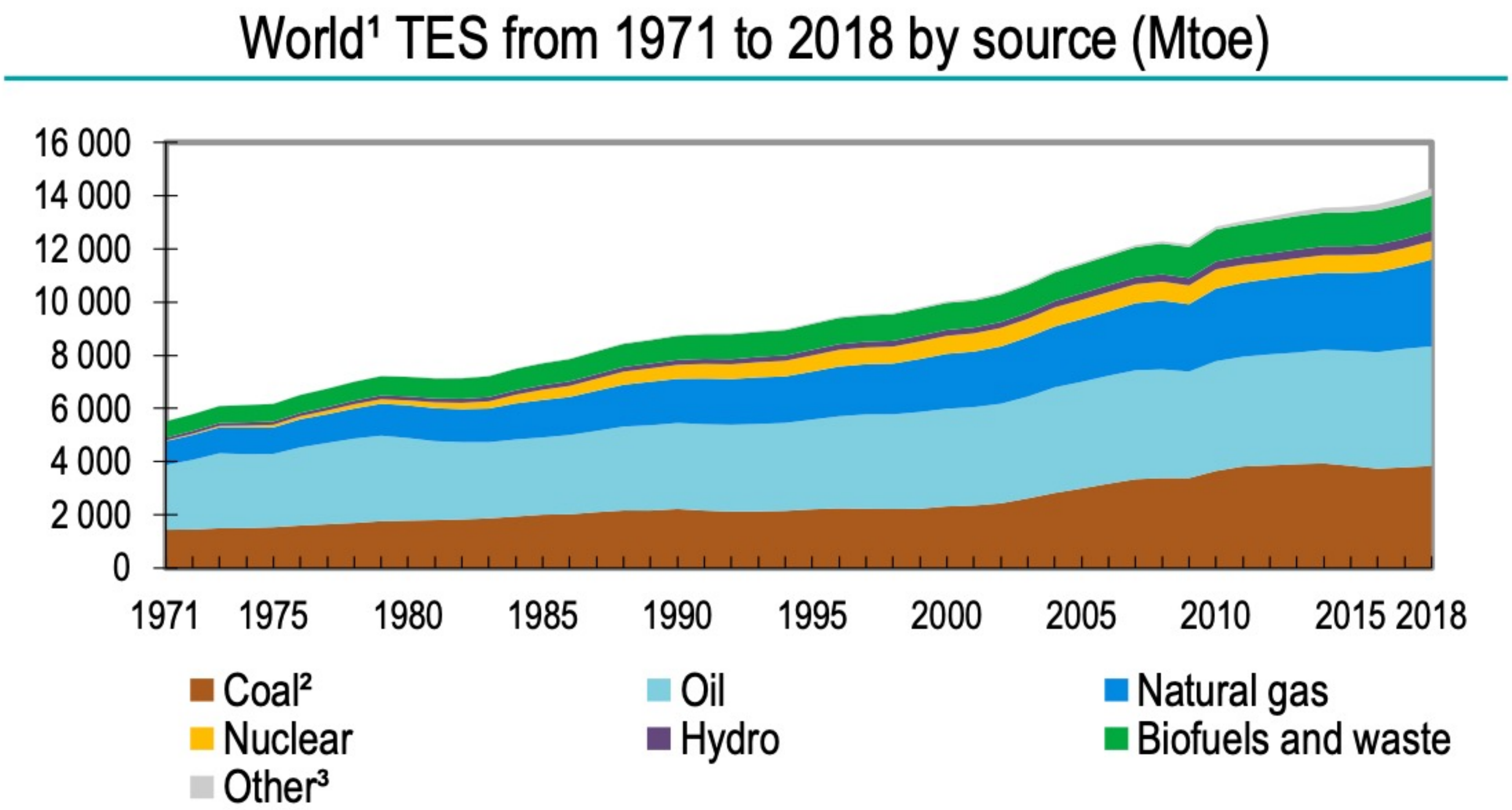

IEA Key stats, 2020

1 ton of oil has 42 GJ

World Primary Energy Supply

IEA Key stats, 2020

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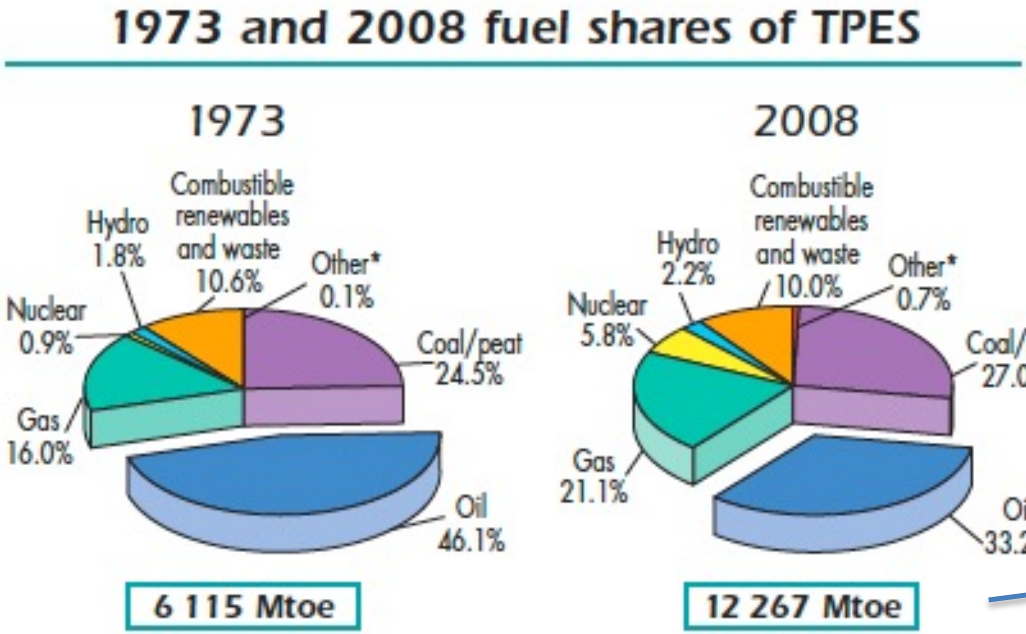
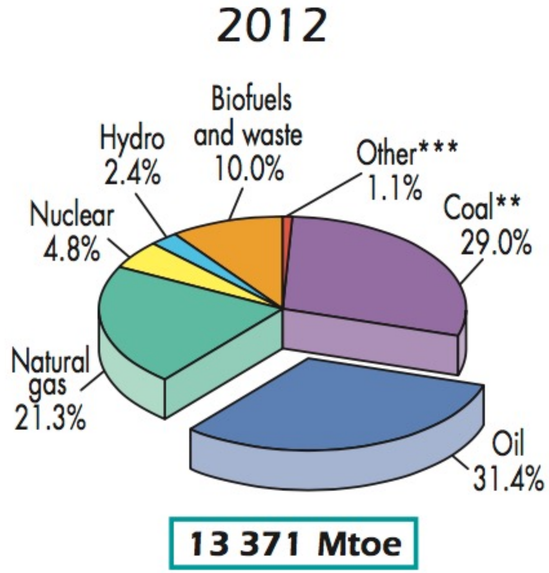
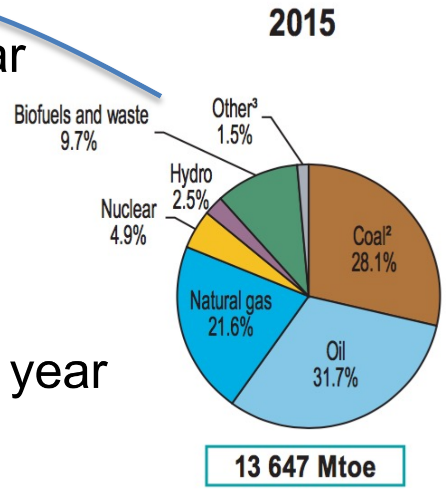
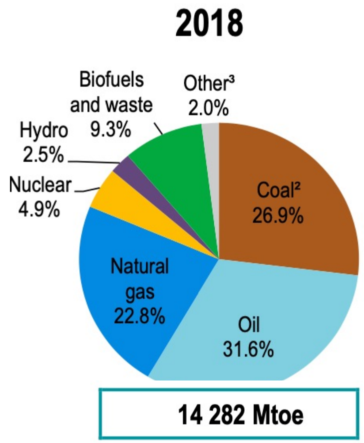




~3% increase per year

~2% increase per year

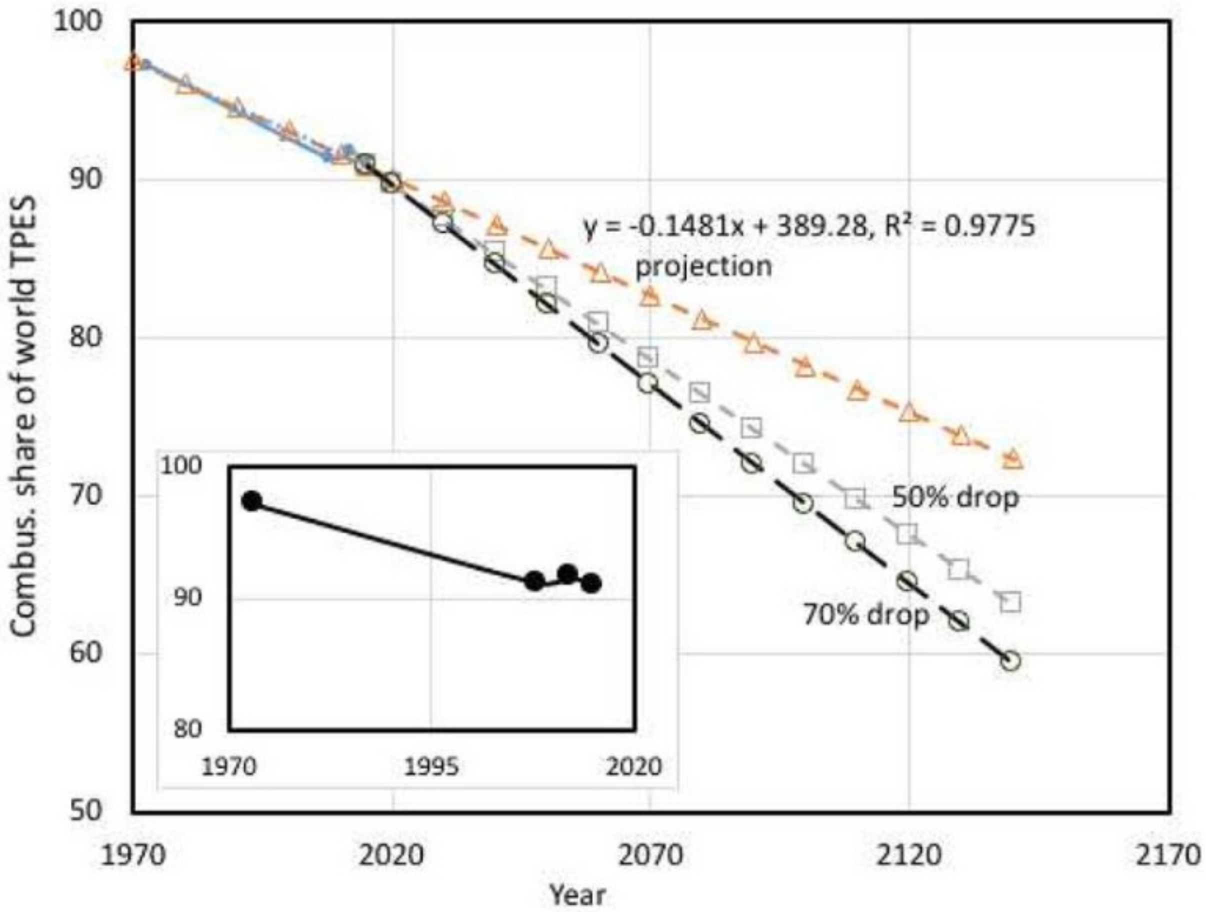




~1.5% per year

Combustion: ~ 90%

Some projections



- Still lot to do in combustion research to make combustion systems better (“greener”)
- Unless a radical paradigm shift happens – “nuclear fusion”
- Non-combustion technology – the message is gloomy or invest more to explore new avenues!!

Ref: Front. Mech. Eng. 5:59. 2019 doi: 10.3389/fmech.2019.00059

Why study combustion?

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- Combustion provides about 85-90% of all the energy we use
- Advantages of fossil fuels regarding energy and power density make them very difficult to replace in the short (50 year) term
- Burning fossil fuels is responsible for the main problems we currently face:
  - Global warming
  - Energy security
- Pollutant emissions, including CO2, can still be made much smaller, with engineering advances

Common combustion modes

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Premixed flame

F, O | Product

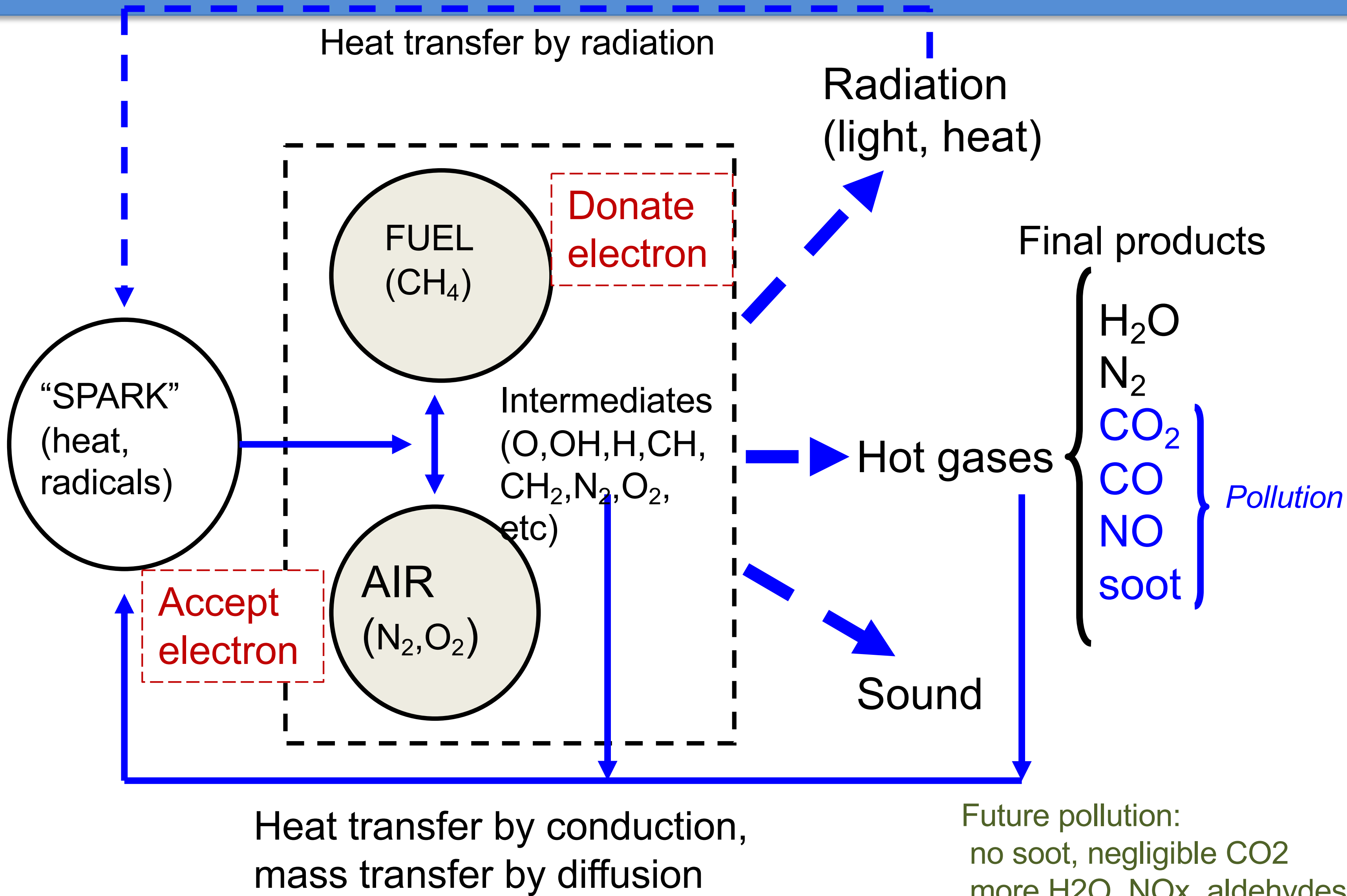
Ex. Spark ignition engines
Stationary GT
a variant for future Aero-GT

Diffusion flame

F | O

Ex. CI engines
Furnaces, Old GTs
Current Aero-GT, after burners
In modern terms – a "dirty flame"

Combustion in a nutshell – relation to other subjects



Future pollution:
no soot, negligible CO2
more H2O, NOx, aldehydes

Objective

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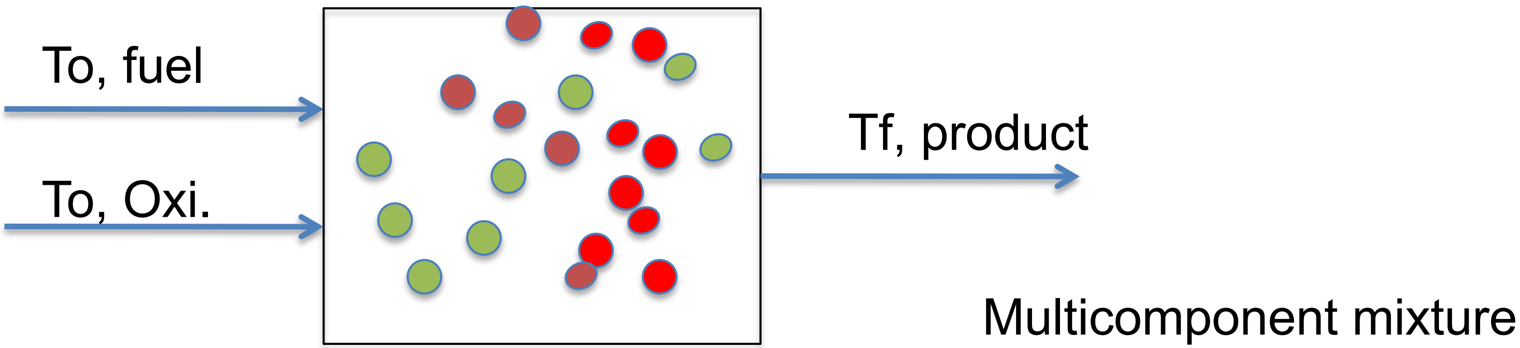

- Introduce concepts to help us to estimate
  - T, composition of products
  - Rate of heat release
  - Ignition energy/T, chemical/thermal explosions
  - Pollutants formation rate
  - Other quantities of interest

Some definitions - Stoichiometry

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Equivalence ratio:

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

ϕ = 1 – Stoichiometric
> 1 – Fuel rich
< 1 – Fuel lean

Air to Fuel ratio:

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

AFR and ϕ are used commonly in combustion analysis

How to get AFR_{st}?

$$C_xH_y + a(O_2 + \frac{0.79}{0.21}N_2) \rightarrow xCO_2 + \frac{y}{2}H_2O + \frac{a0.79}{0.21}N_2$$

Balance of O gives

$$a = x + y/4$$

$$AFR_{st} = \frac{a(MW_{O2} + 0.79/0.21 MW_{N2})}{MW_{fuel}}$$

$$AFR_{st,vol} = \frac{a(1 + 0.79/0.21)}{1}$$

Example

Fuel	CH_4	C_7H_{16}	H_2
c	1	7	0
h	4	16	2
ν_s	2	11	0.5
n_r	10.52	53.4	3.38

total number of moles

$$C_xH_y + a(O_2 + \frac{0.79}{0.21}N_2)$$

Products of Combustion

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$$C_xH_y + \frac{a}{\phi}\left(O_2 + \frac{0.79}{0.21}N_2\right) \rightarrow a_1CO_2 + a_2CO + a_3H_2O + a_4H_2 + a_5O_2 + \frac{a0.79}{\phi 0.21}N_2$$

$\phi = 1$ – Stoichiometric: complete combustion

$$C_xH_y + a\left(O_2 + \frac{0.79}{0.21}N_2\right) \rightarrow xCO_2 + \frac{y}{2}H_2O + \frac{a0.79}{0.21}N_2$$

$\phi < 1$ – Fuel lean – complete combustion

$a_2 = a_4 = 0$

$a_1 = x$, $a_3 = y/2$, and $a_5 = a\boxed{(1-\phi)/\phi}$

Excess air

$\phi > 1$ – Fuel rich

atom conservation is not enough! (more unknown, intermediates, radicals involved)
equilibrium relations are required

Examples

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Example 1 – 1: Calculate the mole and mass fractions in the reactants and products of complete gasoline (taken as 100% octane) combustion at ϕ=0.6 - worked out in Lect. notes (in page 10 of Lect. notes, Ch. 1)

Example 1 – 2: Stoichiometric relations are used to work out molecular composition of fuel and its molecular weight (in page 11 of Lect. notes, Ch. 1)

$$C_xH_yO_o + a(O_2 + 3.76N_2) \rightarrow xCO_2 + \frac{y}{2}H_2O + \frac{a}{\phi}3.76N_2$$

O : $a = x + y/4 - o/2$

Example 1- 2

$$C_xH_yO_o + \frac{a}{\phi}(O_2 + 3.76N_2) \rightarrow a_1CO_2 + a_2H_2O + a_3O_2 + \frac{a}{\phi}3.76N_2$$

4 unknowns

C : $a_1 = x$ H : $a_2 = y/2$ O : $a_3 = a(1-\phi)/\phi$

$$X_{O2,r} = \frac{a/\phi}{1+4.76\,a/\phi} = 0.20807$$

$$p = n_{tot}R^0T$$

$$\frac{n_{tot}^{dry}}{n_{tot}^{wet}} = \frac{p_2T_1}{p_1T_2}$$

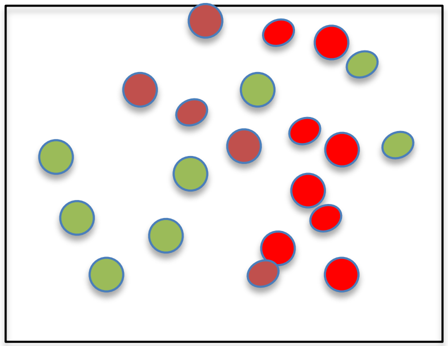
$$X_{O2,p}^{dry} = \frac{a_3}{x + a_3 + 3.76\,a/\phi} = 0.04404$$

$$\frac{n_{tot}^{dry}}{n_{tot}^{wet}} = \frac{x + a_3 + 3.76\,a/\phi}{x + y/2 + a_3 + 3.76\,a/\phi} = \frac{0.517}{0.573}$$

$$X_{CO2,p}^{dry} = \frac{x}{x + a_3 + 3.76\,a/\phi} = 0.12788$$

$$C_{12.6}H_{21.4}O_{1.1} \quad MW = 190 \ \text{kg/kmol}$$

Some definitions



Mole fraction: $X_i = n_i/n_{tot}$ $n_{tot} = \Sigma n_i$ $\sum_{i=1}^{N} X_i = 1$

Mass fraction: $Y_i = m_i/m$ $m = \Sigma m_i$ $\sum_{i=1}^{N} Y_i = 1$

$$Y_i = \frac{m_i}{m} = \frac{n_i MW_i}{n_{tot} \overline{MW}} = X_i \frac{MW_i}{\overline{MW}} \qquad \overline{MW} = \sum X_i MW_i$$

$$C_i = \frac{n_i}{V} = \frac{X_i n_{tot}}{V} = X_i \frac{P}{R^0 T} = Y_i \frac{\rho}{MW_i} \qquad \rho = \sum X_i \rho_i$$

Mean properties: $\eta = \sum_{i=1}^{N} Y_i \eta_i$ $\bar{\eta} = \sum_{i=1}^{N} X_i \bar{\eta}_i$

Adiabatic Flame Temperature

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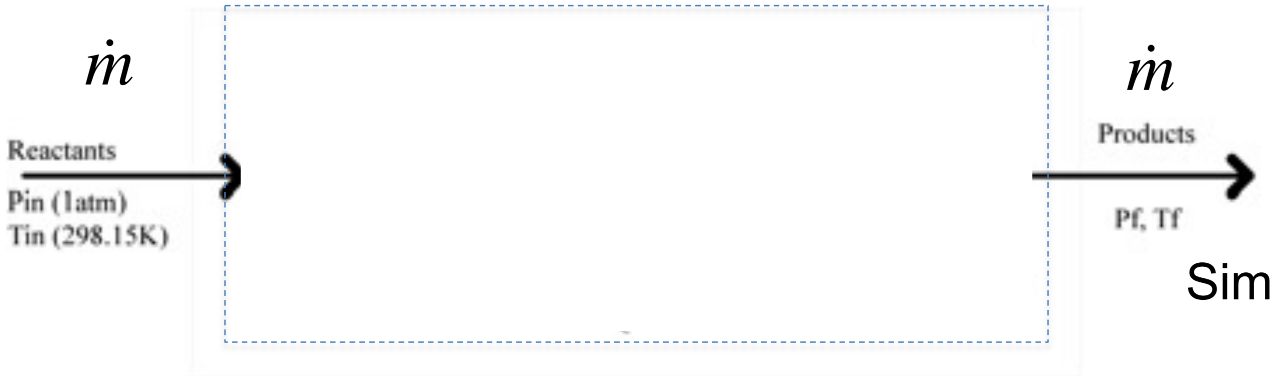


Simple approximation:

$$\dot{m}c_p\left(T_f - T_{in}\right) = \dot{m}_{fuel}Q$$

$$\Rightarrow \quad Y_{fuel}Q = c_p\left(T_f - T_{in}\right)$$

Heat of combustion – Reactants & products are at 298.15K

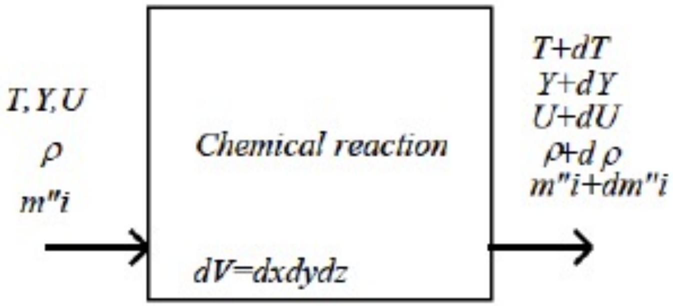
This heat is then used to heat up the products from 298.15 to Tf to satisfy the 1st Law of Thermodynamics

$$\left[\sum_{i=1}^{N} n_i \bar{h}_i(T_{in})\right]_{reac} + Q = \left[\sum_{i=1}^{N} n_i \bar{h}_i(T_f)\right]_{prod}$$

$$\bar{h}_i = \int_{298.15}^{T} \bar{c}_{p,i}\, dT$$

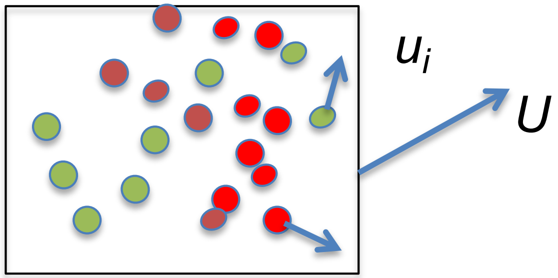
Example 1-3

Conservation equation - Differential



$$\frac{\partial(\rho Y_i)}{\partial t} = -\frac{\partial \dot{m}_i''}{\partial x} + \dot{w}_i$$

summing over all species $\quad \dfrac{\partial \rho}{\partial t} + \dfrac{\partial \rho U}{\partial x} = 0$



$$\dot{m}_i'' = \dot{m}_{i,ADV}'' + \dot{m}_{i,DIFF}''$$

$$\rho U\, Y_i \qquad -\rho\, \mathcal{D}_i \frac{\partial Y_i}{\partial x}$$

$$\mathcal{D}_i = \mathcal{D} \qquad \rho \mathcal{D} = \frac{\lambda}{c_p}$$

$$\frac{\partial \rho\, Y_i}{\partial t} + \frac{\partial \rho U\, Y_i}{\partial x} = \frac{\partial}{\partial x}\left(\rho\, \mathcal{D} \frac{\partial Y_i}{\partial x}\right) + w_i$$

$$\rho\, c_p \frac{\partial T}{\partial t} + \rho\, c_p\, U \frac{\partial T}{\partial x} = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) - Q w_{fuel}$$

Final Note

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$$\frac{\partial \rho Y_i}{\partial t} + \frac{\partial \rho U Y_i}{\partial x} = \frac{\partial}{\partial x}\left(\rho \mathcal{D} \frac{\partial Y_i}{\partial x}\right) + \underline{w_i}$$

Next Lect. : Equilibrium and Chemical Kinetics