Condensed Combustion Notes

https://camillejr.github.io/science-docs/

1 Basic concepts

1.1 Species

Species is a general name for any chemical compound that takes role in a chemical reaction. In the context of combustion the most encountered species are for instance: CO2, CO, H2O, O2, N2, etc.

1.2 Species mass fraction

A species mass fraction is a ratio between mass m_i of a particular i-th species in the mixture and the total mass of the mixture m_{TOT}:

$$Y_i = \frac{m_i}{m_{TOT}} \tag{1}$$

1.3 Species mole fraction

A species molar fraction is the ratio between number of moles N_i of a particular i-th species in the mixture and the total number of moles of the mixture N_{TOT}:

$$\chi_i = \frac{N_i}{N_{TOT}} \tag{2}$$

1.4 Mass-basis and molar-basis quantities

In combustion, we encounter both *mass-basis* and *molar-basis* quantities. According to [2], the mass-basis is useful because mass is conserved and molar-basis is useful because chemical reactions are written per-molar basis.

1.5 Air-to-fuel ratio

Air-to-fuel ratio is the ratio between mass of air m_{air} and mass of fuel m_{fuel} in the mixture.
The stoichiometric air-to-fuel ratio:

$$AF_{st} = \left(\frac{m_{air}}{m_{fuel}}\right)_{st} \tag{3}$$

And a general air-to-fuel ratio for any mixture:

$$AF = \frac{m_{air}}{m_{fuel}} \tag{4}$$

1.6 Equivalence ratio

The equivalence ratio is the ratio between stoichiometric air-to-fuel ratio and an actual air-to-fuel ratio:

$$\phi = \frac{AF_{st}}{AF} \tag{5}$$

When the real mixture has excess air (it is a **lean** mixture), $\phi < 1$. For **rich** mixtures $\phi > 1$.

1.7 Mixture fraction

In general, when we create an unburnt mixture from fuel and oxidizer streams, the *fuel stream* is composed of fuel and other fuel-impurities and the *oxidizer stream* is composed of oxidizer and other oxidizer-impurities. The mass of the total fuel stream is m_1 and the mass of the total oxidizer stream is m_2.
The mixture fraction is the ratio between mass of the fuel stream to the total mass of the unburnt mixture:

$$Z = \frac{m_1}{m_{u,TOT}} = \frac{m_1}{m_1 + m_2} \tag{6}$$

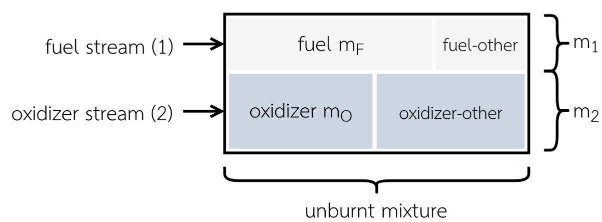

Figure 1: Mixture fraction notion.

We may also define the mass fraction of fuel in the unburnt mixture:

$$Y_{u,F} = \frac{m_F}{m_{u,TOT}} = \frac{m_F}{m_1 + m_2} \tag{7}$$

and mass fraction of fuel in the fuel stream:

$$Y_{1,F} = \frac{m_F}{m_1} \tag{8}$$

These two quantities are clearly related to each other via the mixture fraction:

$$Y_{u,F} = \frac{m_F}{m_1 + m_2} = \frac{m_F}{m_1}\frac{m_1}{m_1 + m_2} = Y_{1,F} Z \tag{9}$$

Similar reasoning can be done for the oxidizer in the oxidizer stream.

1.8 Adiabatic flame temperature

Adiabatic flame temperature is the temperature of combustion products if the combustion happens without heat exchange with the surroundings. It thus has the meaning of maximum possibly achievable temperature for a given combustion.

1.8.1 Constant pressure AdFT

1.8.2 Constant volume AdFT

2 Energy considerations

3 Transfer equations

3.1 Species transport

The mechanical transport of species can happen in twoform: due to a bulk motion of the fluid and/or due to diffusion.

3.1.1 Fick's law

The Fick's law of diffusion states that the mass flow rate is proportional to the concentration gradient with the proportionality constant $-\rho\mathcal{D}$:

$$\frac{d\dot{m}_{diff}}{dA} = -\rho\mathcal{D}\frac{dY}{dx} \tag{10}$$

3.1.2 One-dimensional binary diffusion

For a one-dimensional, binary diffusion (diffusion between two species A and B) we have the mass flow rate of species A per unit area described as:

$$\frac{d\dot{m}_A}{dA} = Y_A\frac{d\dot{m}_{TOT}}{dA} - \rho\mathcal{D}_{AB}\frac{dY_A}{dx} \tag{11}$$

where $\dot{m}_{TOT} = \dot{m}_A + \dot{m}_B$

4 Chemical reactors

A APP1

B APP2

References

[1] S. R. Turns, *An Introduction to Combustion: Concepts and Applications*, Second Edition, 2000

[2] H. Pitsch, *Combustion Theory and Applications in CFD*, Lecture Series