Condensed Combustion Notes

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Preface

These are dense notes on combustion concepts, starting from preliminary notions that are needed in understanding the combustion language, later introducing the elements of thermodynamics relevant to the study of combustion, and finally moving on to the governing differential relations for reactive flows for various systems.
This document is still in preparation.

Contents

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: CO_2, CO, H_2O, O_2, N_2, 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

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:

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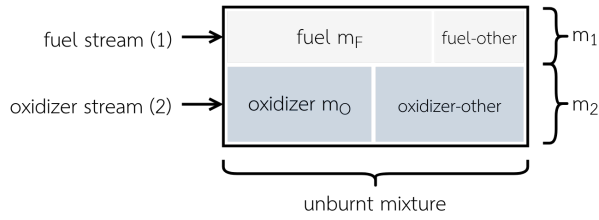

Figure 1: Fuel-oxidizer stream system.

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

2.1 Thermodynamic potentials

2.2 Enthalpy of formation

2.3 First law of thermodynamics

2.4 Second law of thermodynamics

3 Species transport

3.1 1-D species transport

The mechanical transport of species can be twofold: due to a bulk motion of the fluid and/or due to molecular diffusion. Below, we consider one-dimensional binary transport.

3.1.1 1-D diffusion from Fick's law

One way to model molecular diffusion is to use Fick's law. It states that the mass flow rate is proportional to the concentration gradient with the constant $-\rho\mathcal{D}$:

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

In the 1-D case, the quantity $\mathcal{D}$ is called *binary diffusivity* and its units are m^2/s. In the above equation, $\dot{m}_{i,diff}$ is the mass flux of species due to diffusion, ρ is the density and Y is the concentration of species.

3.1.2 1-D bulk flow

The bulk motion of species is simply the portion of the mixture mass flux described by the mass fraction of that species:

$$\frac{d\dot{m}_{i,bulk}}{dA} = Y_i\frac{d\dot{m}_{TOT}}{dA} \tag{11}$$

3.1.3 1-D binary transport

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:

$$\frac{d\dot{m}_A}{dA} = Y_A \frac{d\dot{m}_{TOT}}{dA} - \rho \mathcal{D}_{AB} \frac{dY_A}{dx} \qquad (12)$$

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

3.1.4 1-D species conservation

Differential relations for one-dimensional species conservation can be derived by considering a 1-D control volume Δx. The change of mass of a species A in the control volume can be written as:

$$\frac{dm_{A,CV}}{dt} = \left[\frac{d\dot{m}_A}{dA} A\right]_x - \left[\frac{d\dot{m}_A}{dA} A\right]_{x+\Delta x} + r_A V \qquad (13)$$

where r_A is the mass production rate of species A per unit volume. For further considerations we will call this term the *source term*.

Substituting $m_{A,CV} = Y_A m_{CV} = Y_A \rho A \Delta x$ we get:

$$A\Delta x \frac{d\rho Y_A}{dt} = \left[\frac{d\dot{m}_A}{dA} A\right]_x - \left[\frac{d\dot{m}_A}{dA} A\right]_{x+\Delta x} + r_A A \Delta x \qquad (14)$$

Using the relation for 1-D binary diffusion from eq.(3.1.3), and dividing by $A\Delta x$ we get:

$$\begin{aligned}
\frac{d\rho Y_A}{dt} =& \frac{1}{\Delta x}\left[Y_A \frac{d\dot{m}_{TOT}}{dA} - \rho \mathcal{D}_{AB}\frac{dY_A}{dx}\right]_x \\
&- \frac{1}{\Delta x}\left[Y_A \frac{d\dot{m}_{TOT}}{dA} - \rho \mathcal{D}_{AB}\frac{dY_A}{dx}\right]_{x+\Delta x} \\
&+ r_A
\end{aligned} \qquad (15)$$

Finally taking the limit as $\Delta x \to 0$:

$$\frac{d\rho Y_A}{dt} = -\frac{\partial}{\partial x}\left[Y_A \frac{d\dot{m}_{TOT}}{dA} - \rho \mathcal{D}_{AB}\frac{dY_A}{dx}\right] + r_A \qquad (16)$$

3.2 Source terms

3.3 3-D species transport

We now extend our previous relations to the 3-D case.

3.3.1 Reaction rate considerations

4 Extension to thermal equations

5 Chemical reactors

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