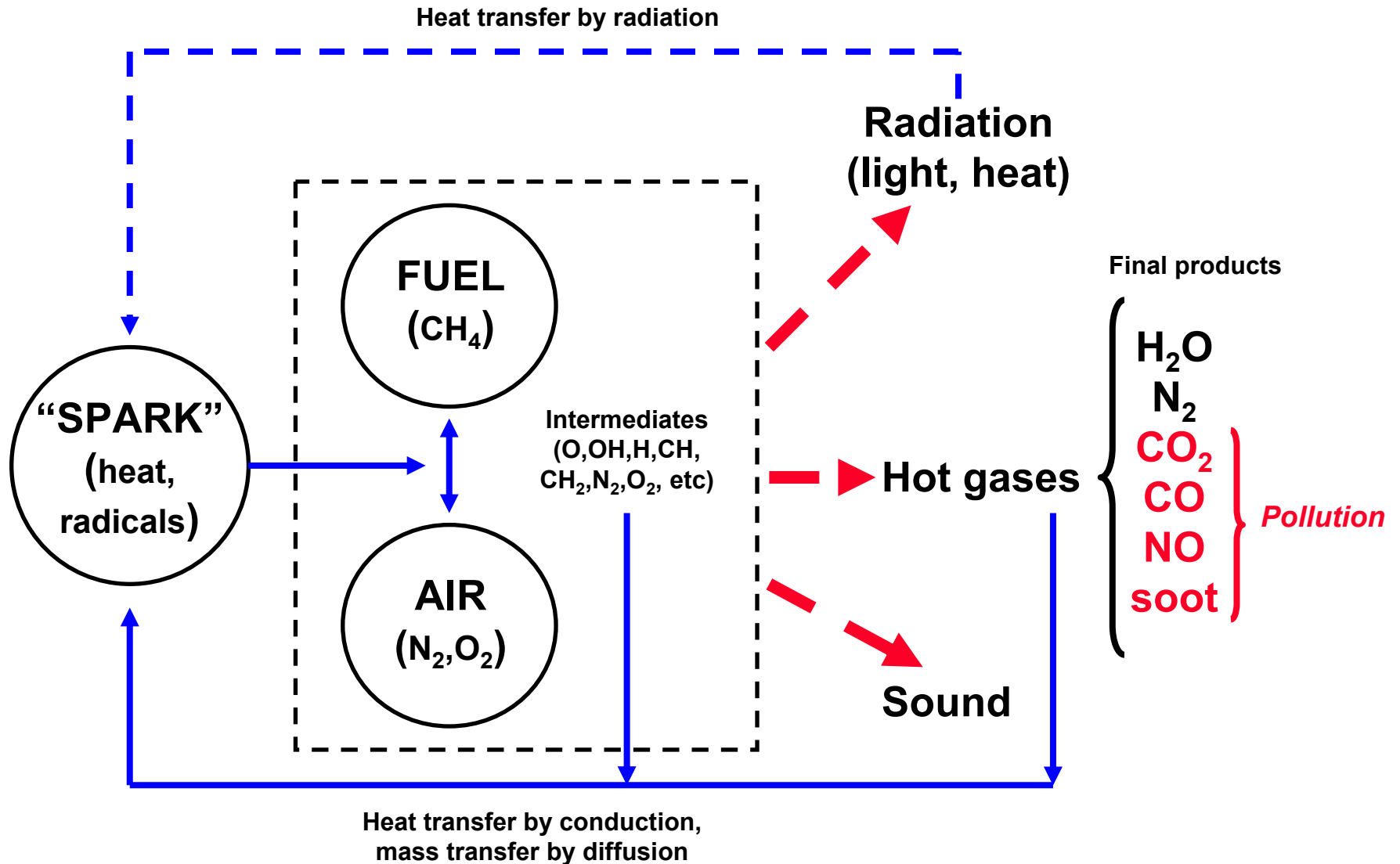


Combustion in a nutshell



Chapter 1: Introduction to Combustion, flame temperature, governing equations

Objectives

The objectives of this Lecture are:

- To introduce the need to study combustion.
- To review various expressions to characterize mixtures.
- To review the calculation of the adiabatic flame temperature for complete combustion.
- To derive simplified governing equations for reacting flow.
- To introduce mass transfer concepts.

Introduction - power from combustion

About 90% of the world's energy comes from the combustion of fossil fuels. Energy is needed for transport (land, sea, air), electricity generation, heating in buildings and industrial processes (e.g. iron, steel, aluminium, paper, cement manufacture). Combustion occurs in boilers, refineries, glass melters, drying kilns, incinerators, industrial ovens and is also used to generate energy from biomass (e.g. from wood, straw, organic waste).

The fuels we use could be in solid, liquid, or gaseous form. Coal, biomass, and municipal waste are mostly solids; oil and its derivatives (gasoline, kerosene, diesel) are liquids; natural gas (mostly methane), propane and hydrogen are gases. The state of the fuel determines to a large extent the combustion technology used, but it is fair to say that most energy-releasing reactions occur in the gaseous phase, and hence these are what we will study in this course.

The downside of fossil fuels - and indeed the major driving force for current combustion research, development and investment, is *environmental pollution*. Here, we will also study the most important pollutants and the techniques used to reduce their generation. The amount of pollutants emitted from most combustion sources is *strictly regulated* by legislation in most of the developed world and forms the topic of political discussion and affects economic decisions. To conform to the legislation, new ideas on how to burn are needed and it is hoped that the student will leave this course more informed about a very serious problem that concerns us all.

Combustion science

Definitions of combustion

Oxford Concise Dictionary gives: 1. Consumption by fire; 2. Development of light and heat with chemical combination. Webster's Dictionary gives: 1. Rapid oxidation generating heat or both light and heat; 2. Slow oxidation accompanied by relatively little heat and no light. Our working definition in this course is that combustion is a "*chemical reaction between fuel and oxidizer involving significant release of energy as heat*". *Fuel* is any substance that releases energy when oxidized (e.g. methane - CH_4 , octane - C_8H_{18}). *Oxidizer* is any oxygen-containing substance (e.g. air) that reacts with fuel. The *reaction* occurs usually in a small fraction of the available volume in the *reaction zone* or *flame*. This is the rapid mode of combustion. Reaction may produce intermediates that chemiluminesce or particles that glow and hence the colour of flames. Combustion may also be occurring close to a catalytic surface at low temperatures: this is the slow mode. The most common type is the rapid form of combustion, i.e. rapid oxidation at high temperatures ($>1500\text{ K}$), and this is the situation we are most interested in for power generation.

Relevance to other subjects

Flames involve fluid motion, diffusion of heat and mass, heat release, and chemistry. Hence, the study of combustion is based on *thermodynamics*, *chemical kinetics*, *heat and mass transfer*, and *fluid mechanics*. Engineers with a good handling of combustion become very competent in all branches of Thermofluids. We will draw analytical techniques from previous courses on (i) Thermodynamics (SFEE, equilibrium); (ii) Fluid Mechanics (control-volume analysis); and (iii) Mathematics (ordinary differential equations). The course also has a significant qualitative component, because it is very difficult to obtain quantitative results for some combustion phenomena without resort to numerical analysis. We mostly seek understanding of combustion physics, rather than exact numerical results.

Revision of basic concepts, new terminology

In combustion, we work with *concentrations*, *mole fractions*, or *mass fractions* according to personal taste or convenience. We are dealing with mixtures of species and we want to be able to calculate various average properties and, in particular, to characterize the fuel-air mixture. We review here all the relevant relations. Most of this material has already been covered in Thermofluids of Part IA and Part IB.

Equivalence ratio

The equivalence ratio of a fuel-air mixture is defined as

$$\phi = \frac{(m_{fuel}/m_{air})}{(m_{fuel}/m_{air})_{st}} = \frac{(V_{fuel}/V_{air})}{(V_{fuel}/V_{air})_{st}}, \quad (1.1)$$

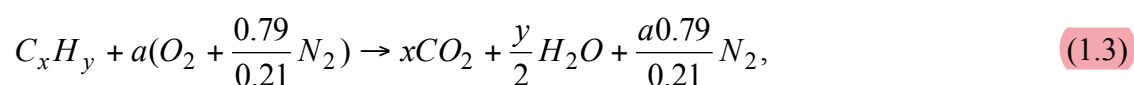
expressed in terms of the mass (m) or volume (V) of fuel and air present in the mixture. The subscript st refers to stoichiometric conditions. The equivalence ratio is related to the Air to Fuel Ratio (AFR) by

$$AFR = \frac{1}{\phi} AFR_{st}. \quad (1.2)$$

Pure fuel corresponds to $AFR=0$ and $\phi=\infty$, while pure air to $AFR=\infty$ and $\phi=0$. In some cases, it is customary to work in terms of the AFR (or $1/\phi$) (e.g. in gas turbines) and in others to work with ϕ (e.g. in SI engines).

Calculation of AFR_{st}

The stoichiometric quantity of oxidizer is just that amount that is necessary to completely burn a quantity of fuel. The stoichiometric AFR is calculated by balancing C, H, and O atoms in the combustion reaction. Complete combustion of a general hydrocarbon with atmospheric air is written as



Each kmol of atmospheric air has 0.79kmol of N_2 and 0.21kmol of O_2 . C, H, and N atom balance have already been enforced in Eq. (1.3). By counting O atoms, it is easy to see that

$$a = x + y/4. \quad (1.4)$$

The stoichiometric AFR (by mass) is then given by

$$AFR_{st} = \frac{a(MW_{O_2} + 0.79/0.21MW_{N_2})}{MW_{fuel}}, \quad (1.5)$$

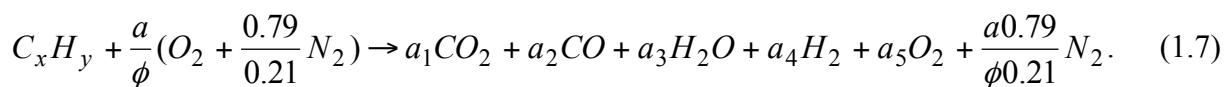
with a given by Eq. (1.4). The volumetric AFR_{st} is given by

$$AFR_{st,vol} = \frac{a(1 + 0.79/0.21)}{1}. \quad (1.6)$$

For example, for CH_4 , $x=1$ and $y=4$, hence $a=2$, and the volumetric $AFR_{st,vol}$ is 9.524, while the mass AFR_{st} is 17.167. If there is no explicit distinction as to whether the AFR refers to mass or volume (molar) ratio, we usually take it as a mass ratio. The same approach can be used to find the stoichiometric ratio of any fuel to any air. For example, the fuel may contain oxygen or nitrogen (e.g. various coals of the generic formula $C_pH_qO_rN_s$), while the O_2/N_2 ratio in the “air” used in combustion may be different from that in atmospheric air, for example due to oxygen enrichment to achieve high temperatures.

Products of combustion

The reaction of *lean* ($\phi < 1$), stoichiometric ($\phi = 1$) or *rich* ($\phi > 1$) mixtures with atmospheric air can be written in the general form:



One could add other species in the r.h.s. (e.g. O, H, OH etc), if required. Equation (1.7) is the starting point in evaluating the composition of the product mixture and it is different from Eq. (1.3).

- For $\phi=1$ and complete combustion, Eq. (1.7) reduces to Eq. (1.3).
- If $\phi < 1$ and complete combustion occurs, $a_2=a_4=0$ (all fuel is oxidized to CO_2 and H_2O) and then atomic balances of C, H, and O give that $a_1=x$, $a_3=y/2$, and $a_5=a(1-\phi)/\phi$. The quantity $(1-\phi)/\phi$ is referred to in the literature as the “*excess air*”.
- If $\phi > 1$, it is not possible to calculate the final product composition simply by atom conservation because CO and H_2 are also present (we get more unknowns than equations). Equilibrium considerations will resolve this in chapter 3.

Mole fractions and mass fractions

The factor that appears before the chemical symbol in the combustion equation (1.3) or (1.7) is the number of kmols of that particular species. The total number of kmols may be different in the products than in the reactants. The ratio of the number of kmols, n_i , of a particular species i to the total number of kmols n_{tot} in the mixture is the *mole fraction* or *volume fraction*:

$$X_i = \frac{n_i}{n_{tot}}. \quad (1.8)$$

The *mass fraction* Y_i is defined as the mass of i divided by the total mass. Using the obvious

$$\sum_{i=1}^N X_i = \sum_{i=1}^N Y_i = 1, \quad (1.9)$$

where N is the total number of species in our mixture, the following can be easily derived for Y_i and the mean molecular weight \overline{MW} :

$$Y_i = X_i \frac{MW_i}{\overline{MW}}, \quad (1.10)$$

$$\overline{MW} = \sum_{i=1}^N X_i MW_i = \left(\sum_{i=1}^N \frac{Y_i}{MW_i} \right)^{-1}. \quad (1.11)$$

Note that the combustion equation (1.3 or 1.7) gives us mole fractions, which can then be used to give mass fractions through the individual and the mean molecular weights.

Concentrations

The *concentration* of species i is defined as the number of kmols of the species per unit volume. The usual notation used for concentrations is C_i or the chemical symbol of the species in square brackets, e.g. $[\text{CH}_4]$ for methane. From this definition and Eq. (1.8),

$$C_i = \frac{n_i}{V} = \frac{X_i n_{tot}}{V}, \quad (1.12)$$

and using the equation of state $PV = n_{tot} R^0 T$ (R^0 is the universal gas constant), we get:

$$C_i = \frac{X_i n_{tot}}{n_{tot} R^0 T / P} = X_i \frac{P}{R^0 T} \quad (1.13)$$

This relates the concentration to the mole fraction. Note that the total pressure P and the temperature T of the mixture have now appeared (i.e. for given mass or mole fractions, the concentrations are functions of pressure and temperature). Applying Eq. (1.10) to Eq. (1.13), we relate the concentration to the mass fraction:

$$C_i = \frac{Y_i \overline{MW}}{MW_i} \frac{P}{R^0 T} = \frac{Y_i \rho}{MW_i}. \quad (1.14)$$

The mixture density ρ appearing in Eq. (1.14) can be related to the mixture constituent densities by

$$\rho = \frac{P \overline{MW}}{R^0 T} = \sum_{i=1}^N \frac{P X_i MW_i}{R^0 T} = \sum_{i=1}^N X_i \rho_i \quad (1.15)$$

where ρ_i is the density of each species calculated at the total pressure. The first equality in Eq. (1.15) constitutes the definition of the mixture density, while the last can be used to get the mean density from Tables that give the individual species densities at a given temperature and pressure. As a (good) first approximation in combustion problems, the mixture molecular weight (and hence density) may be taken as that of air due to the abundance of N_2 , especially for lean mixtures.

Usually, the chemical reaction rate is expressed in terms of concentrations, while the conservation laws for mass, momentum, and energy that are used in combustion problems are expressed in terms of mass fractions. On the other hand, it is the volume fractions that are measured (e.g. by exhaust gas analysers) or set (e.g. by flow meters) in practice. The above relations are useful for performing transformations between the various quantities.

Intensive mixture properties

Thermodynamic properties may be reported on a molar or a mass basis. For example, enthalpy could be in kJ/kmol or in kJ/kg. **Molar quantities are denoted by an overbar.** Hence the enthalpy h_i for each species i and for the whole mixture are given by:

$$h_i = \bar{h}_i / MW_i \quad (1.16)$$

$$h = \sum_{i=1}^N Y_i h_i \quad (1.17)$$

$$\bar{h} = \sum_{i=1}^N X_i \bar{h}_i = h \bar{MW} \quad (1.18)$$

Equations (1.17) and (1.18) are the definitions for the mixture enthalpies. The SFEE can be written in terms of h or \bar{h} . Similarly for internal energies.

Heat of combustion and adiabatic flame temperature

The heat of combustion was defined as the heat released per unit mass of fuel when stoichiometric reactants (fuel + air) burn and both the reactants and the products are at 298.15K and 1atm. The concept is illustrated in the control volume analysis of Fig. 1-1. To calculate the flame temperature after the reaction we resort to a two-stage analysis. First, the reaction occurs at 298.15K, an amount of heat is released which is calculated based on the amount of fuel and the heat of combustion, and then this heat is used to raise the temperature of the products from 298.15K to the final temperature. From values of enthalpies (e.g. in Thermofluids Data Book), we are in a position to calculate the temperature at which the total enthalpy rise is equal to the heat released by combustion and hence to find the final products temperature. In other words, we seek the temperature T_f such that the First Law is satisfied:

$$\left[\sum_{i=1}^N n_i \bar{h}_i(T_{in}) \right]_{reac} + Q = \left[\sum_{i=1}^N n_i \bar{h}_i(T_f) \right]_{prod} \quad (1.19)$$

n_i is the number of kmol and \bar{h}_i is the molar enthalpy of species i . The summation is done over all species present in the reactants or the products. T_f will decrease if there is heat loss from the system, if T_{in} is less than 298.15K, or if there is phase change, e.g. when some of the heat released must be used for evaporation. Using Eq. (1.19) is a little cumbersome to use, as it requires looking up values of enthalpy.

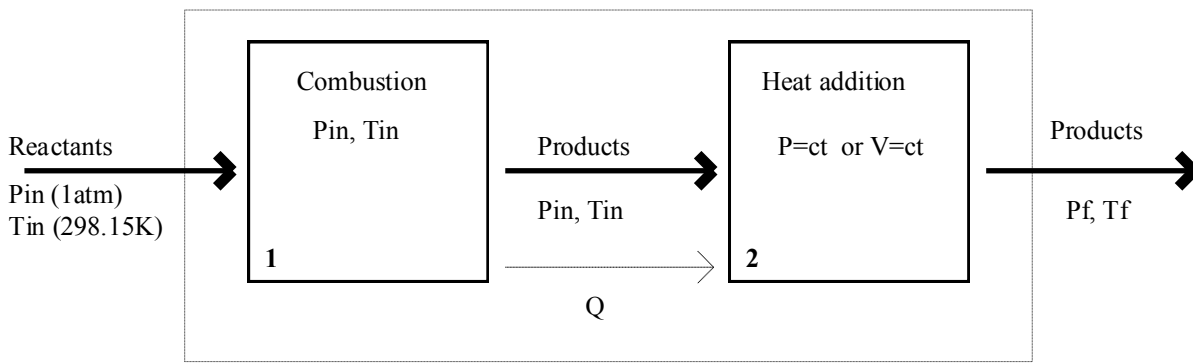


Figure 1-1 Control volume analysis for the calculation of adiabatic flame temperatures. If $P_{in}=1$ atm and $T_{in}=298.15\text{K}$, then Q is defined as the “heat of combustion”.

Approximations to T_f

The approach above provides an exact calculation for the adiabatic flame temperature. To obtain an approximate but simple estimate for T_f , we will assume constant c_p . Then, we have for constant pressure

$$Y_{fuel}Q = c_p(T_f - T_{in}) \quad (1.20)$$

that essentially says that all the heat released by the combustion ends up as sensible enthalpy of the products. Equation (1-20) is very useful, but not very accurate if c_p is based on T_{in} . We can increase accuracy if an average value of c_p , corresponding to air at $(T_{in}+T_f)/2$, is used. Equation (1.20) with c_v replacing c_p can be used to obtain a rough estimate to the constant-volume adiabatic flame temperature. We will use Eq. (1.20) extensively in this course.

Governing equations for reacting flow

Conservation of mass

Consider an infinitesimal control volume ΔV (Fig. 1-2). Inside the CV we have a uniform mixture of species undergoing chemical reactions. Mass may cross the surfaces of the CV. For simplicity of presentation we assume a one-dimensional geometry. Then, the principle of mass conservation of each species i reads:

$$\begin{aligned} [\text{Rate of accumulation}] &= [\text{Rate at which species comes in}] - [\text{Rate at which species leaves}] \\ &+ [\text{Rate of generation due to reaction}] \end{aligned}$$

In mathematical terms,

$$\frac{\partial(m_V Y_i)}{\partial t} = \dot{m}_i'' \Delta y \Delta z - (\dot{m}_i'' + \Delta \dot{m}_i'') \Delta y \Delta z + \dot{w}_i \Delta V \quad (1.21)$$

with the following definitions:

m_V	(kg)	total mass of mixture inside the control volume, $m_V = \rho \Delta x \Delta y \Delta z$
Y_i	(-)	mass fraction of i

ρ	(kg m ⁻³)	mixture density
\dot{m}_i''	(kg m ⁻² s ⁻¹)	mass flow of species i per unit time per unit surface, the <i>mass flux</i>
\dot{w}_i	(kg m ⁻³ s ⁻¹)	mass of i generated per unit volume per unit time due to chemical reactions

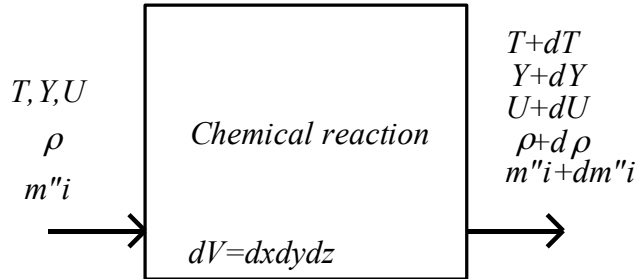


Figure 1-2 Control volume for derivation of species conservation and temperature equation.

Letting Δx go to zero, we obtain the *species conservation equation*:

$$\frac{\partial(\rho Y_i)}{\partial t} = -\frac{\partial \dot{m}_i''}{\partial x} + \dot{w}_i \quad (1.22)$$

Equation (1.22) is a partial differential equation (in time and space) and to be in a position to solve it, we need expressions for the mass flux and the rate of generation due to chemistry. We will consider the mass flux here and the reaction rate in chapter 2.

The sum of mass fluxes of all species is the *total mass flux* \dot{m}'' (kg m⁻² s⁻¹), which we recognize from fluid mechanics courses as

$$\dot{m}'' = \sum_{i=1}^N \dot{m}_i'' = \rho U \quad (1.23)$$

with U the mixture velocity. No net mass can be generated by the reaction (the reaction transforms one species to another, it does not create mass), and hence

$$\sum_{i=1}^N \dot{w}_i = 0 \quad (1.24)$$

Using Eqs. (1.23) and (1.24) and summing Eq. (1.22) over all species, we obtain the well known *continuity equation* of fluid mechanics:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho U)}{\partial x} = 0 \quad (1.25)$$

Therefore a multi-component mixture obeys the same mass conservation equation as a simple fluid (1.25), and each constituent species obeys its own conservation equation (1.22).

Mass flux, mass transfer and Fick's Law of diffusion

The mass flux \dot{m}_i'' for each species that appears in the species conservation equation is composed of two parts: an *advective* and a *diffusive* part. This result is given here without proof, as it can be proven from the Kinetic Theory of Gases (Part IIB).

$$\dot{m}_i'' = \dot{m}_{i,ADV}'' + \dot{m}_{i,DIFF}'' \quad (1.26)$$

The advective mass flux is due to the bulk fluid motion and is given by:

$$\dot{m}_{i,ADV}'' = Y_i \dot{m}'' = Y_i \rho U \quad (1.27)$$

For the purposes of this course, the diffusive mass flux is given by *Fick's Law*:

$$\dot{m}_{i,DIFF}'' = -\rho D_i \frac{\partial Y_i}{\partial x} \quad (1.28)$$

Fick's Law states that the mass flux is proportional to the gradient of the mass fraction of the species. This is a diffusion process because it tends to make concentration gradients more uniform, i.e. it mixes the various species together. The coefficient D_i ($\text{m}^2 \text{s}^{-1}$) is the *diffusion coefficient* and, in general, depends on the nature of the diffusing species and the nature of the species it diffuses into, i.e. D_i is really a function of the whole mixture. It is a good approximation, however, to take $D_i = D$ to be the same for all species. For simplicity, we will further assume that it is constant. It is also a common approximation that the diffusion of heat and mass follow the same rate, i.e. D is related to the conductivity λ :

$$\rho D = \frac{\lambda}{c_p} \quad (1.29)$$

The non-dimensional number $\lambda/\rho D c_p$ is called the Lewis number Le . Eq. (1.29) implies that $Le=1$, and we will use this throughout the course, as it is a common assumption in combustion. Therefore from tabulated values of conductivity we can estimate D .

Final species conservation equation

With these expressions, the species conservation equation takes the final form:

$$\frac{\partial(\rho Y_i)}{\partial t} + \frac{\partial(\rho U Y_i)}{\partial x} = \frac{\partial}{\partial x} \left(\rho D \frac{\partial Y_i}{\partial x} \right) + \dot{w}_i \quad (1.30)$$

The first term in the l.h.s. corresponds to accumulation of species i , the second to advection by the bulk fluid motion, the first term in the r.h.s. corresponds to diffusion and the last to the generation by chemical reactions. It is easy to see that summing Eq. (1.30) over all species results in the continuity equation (1.25).

Conservation of energy

Consider again the CV shown in Fig. 1-2. The First Law states that

$$\begin{aligned} [\text{Rate of accumulation of energy}] &= [\text{Net heat flux (= Convection + Conduction)}] \\ &+ [\text{Rate of heat release due to reaction}] \end{aligned}$$

For low Mach number flows with negligible contribution of the kinetic and gravitational energy to the total energy of the fluid, and assuming equal diffusivities and $Le=1$, the principle of conservation of energy, with our standard assumption of constant c_p , is written as:

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p U \frac{\partial T}{\partial x} = \frac{\partial P}{\partial t} + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) - Q \dot{w}_{fuel} \quad (1.31)$$

This is given here without proof - the proof is very involved and adds little to physical understanding at this stage. Let us explore Eq. (1.31). The first term in the l.h.s., the unsteady term, is the net rate of temperature rise. The second term in the l.h.s. describes *convection* (as in the Heat Transfer course in Part IB). The first term in the r.h.s. is heating (reversible work) due to *compression* and is important for internal-combustion engines. This term is zero if the pressure is constant. The second term in the r.h.s. is due to *heat conduction* and the last term is the *heat released* by combustion (the minus sign is because the \dot{w} for fuel is negative – fuel is consumed). Eqs. (1.30) and Eq. (1.31) will be the starting points in the next Lectures and we will use them in much simpler forms. They are the conservation equations for reacting fluids, whether the fluid is moving or not, uniform or not etc. In general, the p.d.e.'s have additional dimensions (dependencies in y and z), but we will limit our attention to one-dimensional flames. It is very important to have a clear understanding of the various contributions to the energy balance.

Through the developments above:

- The concepts of species and energy conservation for a reacting flow have been introduced.
- Mass transfer due to diffusion has been quantified by Fick's Law (Eq. 1.28).
- Equations (1.30) and (1.31) include various assumptions, but describe quite adequately all the physical phenomena we will be studying.

Summary of main points

- The basic quantities used to characterize a multi-component mixture and the expressions used to relate concentration, mole and mass fraction were reviewed and the equivalence ratio was defined (Eq. 1.1).
- The composition of products of complete combustion was calculated (Eq. 1.7).
- A useful estimate for the constant-pressure T_f is given by Eq. (1.20).
- The species conservation equation has been derived (Eq. 1.30). It is related to the continuity equation of Fluid Mechanics.
- The mass flux is composed of an advective and a diffusive part, the former given by $Y_i \rho U$ and the latter by Fick's Law (Eq. 1.28).
- The energy equation has been presented and the physical significance of each term has been discussed (Eq. 1.31).

Suggested reading

Turns:

Ch. 1 and Ch. 2 (until "Equilibrium").

Ch. 3 (Fick's Law).

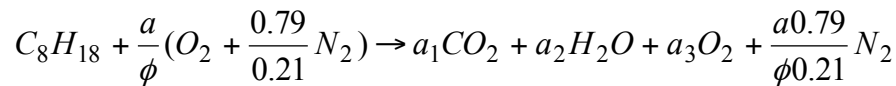
Glassman:

Ch. 1 (pp. 1-7).

Worked examples

Example 1-1. Calculate the mole and mass fractions in the reactants and products of complete gasoline (taken as 100% octane) combustion at $\phi=0.6$.

Assuming complete lean combustion, Eq. (1.7) becomes:



Atom balances give $a=8+18/4=12.5$; $a_1 = 8$; $a_2 = 9$; $a_3 = a(1-\phi)/\phi = 8.333$. The mole fractions in the reactants are:

$$X_{C_8H_{18}} = 1/(1+12.5/0.6+12.5 \cdot 0.79/0.6/0.21) = 0.00998$$

$$X_{O_2} = 0.21 \cdot (1 - X_{C_8H_{18}}) = 0.2079$$

$$X_{N_2} = 0.79/0.21 \cdot X_{O_2} = 0.7821$$

The mean molecular weight of the reactants mixture is

$$0.00998 \cdot 114.23 + 0.2079 \cdot 31.999 + 0.7821 \cdot 28.013 = 29.70 \text{ kg/kmol}$$

and hence the mass fractions are:

$$Y_{C_8H_{18}} = X_{C_8H_{18}} \cdot 114.23/29.70 = 0.0384$$

$$Y_{O_2} = X_{O_2} \cdot 31.999/29.70 = 0.2239$$

$$Y_{N_2} = X_{N_2} \cdot 28.013/29.70 = 0.7377$$

Similarly for the products:

$$X_{CO_2} = 8 / (8+9+8.333+78.373) = 0.0771$$

$$X_{H_2O} = 9 / (8+9+8.333+78.373) = 0.0868$$

$$X_{O_2} = 8.333 / (8+9+8.333+78.373) = 0.0804$$

$$X_{N_2} = 0.7557 \text{ (from the balance)}$$

$$MW_{prod} = 0.0771 \cdot 44.011 + 0.0868 \cdot 18.016 + 0.0804 \cdot 31.999 + 0.7557 \cdot 28.013 = 28.699 \text{ kg/kmol}$$

and then

$$Y_{CO_2} = 0.0771 \cdot 44.011 / 28.699 = 0.1182$$

$$Y_{H_2O} = 0.0868 \cdot 18.016 / 28.699 = 0.0545$$

$$Y_{O_2} = 0.0804 \cdot 31.999 / 28.699 = 0.0896$$

$$Y_{N_2} = 0.7377 \text{ (from the balance)}$$

Notes:

- Nitrogen does not participate in the reactions and hence its mass fraction before and after combustion does not change. There is a change in the total number of moles between the reactants and the products, however, and hence its mole fraction before and after the reaction is different.
- The mean molecular weight is very close to that of air. This is typical of combustion problems.
- The very small fuel mole fraction in the reactants results in a quite substantial mass fraction due to the high molecular weight of octane relative to that of air.



Example 1-2. How does one determine the elemental composition of a complex fuel, such as crude oil, biofuel or wood? The most straightforward way is to burn it. Consider the following experiment, in which a fuel of composition $C_xH_yO_o$ has been burned in a closed vessel of fixed volume, and the reactant and product molar fractions of oxygen and carbon dioxide have been measured on a dry basis after by cooling and condensing the water in the products. The results are

Oxygen mole fraction in reactant is 0.20807

Oxygen mole fraction in dry product is 0.04404

CO₂ molar fraction in dry product is 0.12788

The total number of moles in the product can be obtained by considering the pressures and temperatures of the product mixture as it cools above and below the dew point. Let us call state 1 as the state with all water present as vapour at p_1 and T_1 , and state 2 after all products have condensed at p_2 and T_2 . The ratio p_2/p_1 is 0.517 and $T_2/T_1 = 0.573$.

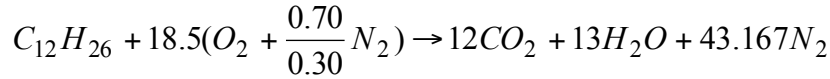


Determine the molecular composition of the fuel and its molecular weight.

Ans: $x = 12.6, y = 21.4, o = 1.1 \Rightarrow C_{12.6}H_{21.4}O_{1.1} \quad MW = 190 \text{ kg/kmol}$

Example 1-3. Calculate the constant-pressure adiabatic flame temperature of diesel fuel (taken as n-dodecane) burning with oxygen-enriched air of composition 30% O₂ and 70% N₂ (by vol.) at $\phi=1$. Assume complete combustion, $P_{in}=P_f=1$ atm and $T_{in}=298$ K. Take $Q=44,467$ kJ/kg.

The complete stoichiometric combustion equation for diesel with our oxygen-enriched air is:



Equation (1.19) gives

$$Q + \left[\sum_{i=1}^N n_i \bar{h}_i(298) \right]_{react} - 12\bar{h}_{CO_2}(T_f) - 13\bar{h}_{H_2O}(T_f) - 43.167\bar{h}_{N_2}(T_f) = 0 \quad (1.32)$$

Neglecting the difference between 298 and 298.15K, $\bar{h}_i(298)=0$ and the term in square brackets goes to zero. Using $Q=44,467$ kJ/kg \cdot 170.337 kg/kmol = 7,574,375 kJ/kmol for diesel, successive guesses for the temperature and reading the enthalpy values from Tables until Eq. (1.32) is satisfied gives that $T_f=3030$ K (by extrapolating from 2900 and 3000K).

To have a quick estimate for T_f , one could assume constant c_p . Then, using $c_p = 1.01$ kJ/kgK (for air), we have (Eq. 1.20):

$$\begin{aligned} Y_{fuel}Q &= c_p(T_f - T_{in}) \\ \Leftrightarrow \frac{MW_{fuel}}{MW_{fuel} + 18.5MW_{O_2} + 43.167MW_{N_2}}Q &= c_p(T_f - T_{in}) \\ \Leftrightarrow T_f &= 3506K \end{aligned}$$

Notes:

- For *atmospheric* air, the kmols of N₂ in the products would be $18.5 \cdot 0.79 / 0.21 = 69.595$. The same calculation with atmospheric air gives $T_f = 2411$ K. Significantly higher temperatures can therefore be achieved with oxygen enrichment, something used quite often in practice if very high temperatures are needed.
- If the mixture were lean, some O₂ and more N₂ would appear in the products and hence the temperature would be lower.
- The two methods of finding the adiabatic flame temperature can be used to define an average c_p . The average c_p for this problem would be $c_p(298) \frac{(3506 - 298)}{(3030 - 298)} = 1.19$ kJ/kgK, an approximately 20% increase from room temperature.
- At high temperatures, dissociation of CO₂ and H₂O occurs which changes the products composition. This causes the temperature to be lower by several hundred K. The present procedure is exact, but the result is inaccurate because the product composition, if we assume complete combustion, is inaccurate. More on this in chapter 3.